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SAMUEL H. MEGERDITCHIAN

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CRYSTALS OF DPP-IV

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December 6, 2004

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Attached please find the certified copies of the foreign application from which priority is claimed for this case:

Country

Application No.

Filing Date

Europe

02026367.9

November 25, 2002

Respectfully submitted,

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The attached documents are exact copies of the European patent application described on the following page, as originally filed.

Les documents fixés à cette attestation sont conformes à la version initialement déposée de la demande de brevet européen spécifiée à la page suivante.

Patentanmeldung Nr.

Patent application No. Demande de brevet n°

02026367.9

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Bezeichnung der Erfindung/Title of the invention/Titre de l'invention: (Falls die Bezeichnung der Erfindung nicht angegeben ist, siehe Beschreibung. If no title is shown please refer to the description. Si aucun titre n'est indiqué se referer à la description.)

Crystal structure of DPP-IV and its use

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Case 21491

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Crystal Structure of DPP-IV and its use

The present invention relates to crystal structure information obtained from crystals of the dipeptidyl-peptidase DPP-IV, to methods of preparing such crystals, and to their use for the identification and/or design of inhibitors of DPP-IV activity. A further subject matter of the invention are methods for the identification and/or design of inhibitor compounds of DPP-IV activity, the inhibitor compounds of DPP-IV activity identified by these methods and their use in pharmaceutical compositions for the treatment and/or prevention of diseases comprising diabetes types I and II, IGT and obesity.

Dipeptidyl peptidase (DPP-IV; T-cell activation antigen CD26 or adenosine binding protein) is a multifunctional type II cell surface glycoprotein. The protein is widely expressed in a variety of cell types, particularly on differential epithelial cells of the intestine, liver, prostate tissue, corpus luteum, and kidney proximal tubles (Hartel, S., Gossrau, R., Hanski, C. & Reutter, W. (1988). Dipeptidyl peptidase (DPP) IV in rat organs. Comparison of immunohistochemistry and activity histochemistry. Histochemistry 89, 151-161; McCaughan, G.W., Wickson, J.E., Creswick, P.F. & Gorrell, M.D. (1990). Identification of the bile canalicular cell surface molecule GP110 as the ectopeptidase dipeptidyl peptidase IV: an analysis by tissue distribution, purification and N-terminal amino acid sequence. Hepatology 11, 534-544) as well as leukocyte subsets (Gorrell, M.D., Wickson, J. & McCaughan, G.W. (1991). Expression of the rat CD26 antigen (dipeptidyl peptidase IV) on subpopulations of rat lymphocytes. Cell. Immunol. 134, 205-215), such as T-helper lymphocytes, and subsets of macrophages (Bühling, F., Kunz, D., Reinhold, D., Ulmer, A.J., Ernst, M., Flad, H.D. & Ansorge, S. (1994). Expression and functional role of dipeptidyl peptidase IV (CD26) on human natural killer cells. Nat. Immun. 13, 270-279) and a soluble form is reported to be present in plasma and urine (Iwaki-Egawa, S.,

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Watanabe, Y., Kikuya, Y. & Fujimoto, Y. (1998). Dipeptidyl peptidase IV from human serum: purification, characterization, and N-terminal amino acid sequence. *J. Biochem.* 124, 428-433). Human DPP-IV has a short cytoplasmatic tail of six amino acids, a 22 amino acid hydrophobic transmembrane region and a 738 amino acid extracellular domain with ten potential glycosylation sites (Tanaka, T., Camerini, D., Seed, B., Torimoto, Y., Dang, N.H., Kameoka, J., Dahlberg, H.N., Schlossman, S.F. & Morimoto, C. (1992). Cloning and functional expression of the T cell activation antigen CD26. *J. Immunol.* 149, 481-486).

DPP-IV is involved in many biological processes, including a membrane-anchoring function for the localization of the extracellular enzyme adenosine deaminase (ADA) 10 (Franco, R., Valenzuela, A., Lluis, C. & Blanco, J. (1998). Enzymatic and extraenzymatic role of ecto-adenosine deaminase in lymphocytes. Immunol. Rev. 161, 27-42), participation in cell matrix adhesion by binding to collagen and fibronectin (Loster, K., Zeilinger, K., Schuppan, D. & Reutter, W. (1995). The cysteine-rich region of dipeptidyl peptidase IV (CD 26) is the collagen-binding site. Biochem. Biophys. Res. Commun. 217, 15 341-348), interaction as a co-receptor for the HIV envelope protein gp 120 (Ohtsuki, T., Tsuda, H. & Morimoto, C. (2000). Good or evil: CD26 and HIV infection. J. Dermatol. Sci. 22, 152-160) and co-stimulatory function during T-cell activation and proliferation (von Bonin, A., Huhn, J. & Fleischer, B. (1998). Dipeptidyl-peptidase IV/CD26 on T cells: analysis of an alternative T-cell activation pathway. Immunol. Rev. 161, 43-53) by interaction with the protein tyrosine phosphatase (CD45) (Torimoto, Y., Dang, N.H., Vivier, E., Tanaka, T., Schlossman, S.F. & Morimoto, C. (1991). Coassociation of CD26 (dipeptidyl peptidase IV) with CD45 on the surface of human T lymphocytes. J. Immunol. 147, 2514-2517).

DPP-IV (EC 3.4.14.5) has postproline dipeptidyl amino peptidase activity, preferentially cleaving X-proline or X-alanine dipeptides from the N-terminus of polypeptides (Hopsu-Havu, V.K. & Glenner, G.G. (1966). A new dipeptide naphthylamidase hydrolyzing glycyl-prolyl-beta-naphthylamide. *Histochemie* 7, 197-201.) and belongs to the prolyl oligopeptidase family, a group of atypical serine proteases able to hydrolyse the prolyl bond (Cunningham, D.F. & O'Connor, B. (1997). Proline specific peptidases. *Biochim. Biophys. Acta* 1343, 160-186). It possesses a novel orientation of its catalytic triad residues (Ser-Asp-His) (Ikehara, Y., Ogata, S. & Misumi, Y. (1994). Dipeptidyl-peptidase IV from rat liver. *Methods Enzymol.* 244, 215-227.), inverse to that found in classical serine proteases (His-Asp-Ser). The cleavage of N-terminal peptides with Pro in the second position is a rate limiting step in the degradation of peptides. The natural substrates of DPP-IV include several chemokines, cytokines, neuropeptides, circulating hormones and bioactive peptides (Lambeir, A.M., Durinx, C., Proost, P., Van

Damme, J., Scharpe, S. & De Meester, I. (2001). Kinetic study of the processing by dipeptidyl-peptidase IV/CD26 of neuropeptides involved in pancreatic insulin secretion. *FEBS Lett.* 507, 327-330.). The wide range of substrates suggests a key regulatory role in the metabolism of peptide hormones and in amino acid transport (Hildebrandt, M., Reutter, W., Arck, P., Rose, M. & Klapp, B.F. (2000). A guardian angel: the involvement of dipeptidyl peptidase IV in psychoneuroendocrine function, nutrition and immune defence. *Clin Sci* 99, 93-104). Its physiological relevance has been investigated by (Hinke, S.A., Pospisilik, J.A., Demuth, H.U., Mannhart, S., Kuhn-Wache, K., Hoffmann, T., Nishimura, E., Pederson, R.A. & McIntosh, C.H. (2000). Dipeptidyl peptidase IV (DPIV/CD26) degradation of glucagon. Characterization of glucagon degradation products and DPIV-resistant analogs. *J. Biol. Chem.* 275, 3827-3834).

The finding that DPP-IV is responsible for more than 95% of the degradation of GLP-1 led to an elevated interest in inhibition of this enzyme for the treatment of diabetes type II. Experiments in rats and humans have provided evidence that specific DPP-IV inhibition increased C_{max} , $T_{1/2}$ and total circulating GLP-1 and decreased plasma glucose. It has been demonstrated that patients with impaired glucose-tolerance (IGT), type-II diabetes and with a secondary failure to respond to sulfonylurea treatment benefit from increased levels of GLP1 peptides. In addition GLP-1 is effective in type-I diabetic patients due to its glucagono-static effect. More recent investigations show a delay of gastric emptying that could have beneficial effects on satiety and might be relevant for the treatment of obesity. Protection of functional GLP-1 by inhibition of DPP-IV and concomitant activation of the GLP-1 receptor might therefore have a synergistic potential in anti-diabetic drug research (Holst, J.J. & Deacon, C.F. (1998). Inhibition of the activity of dipeptidyl-peptidase IV as a treatment for type 2 diabetes. Diabetes 47, 1663-1670.). Selective and orally available small molecule inhibitors of DPP-IV have been discovered and are now in clinical trials (Villhauer, E.B., Brinkman, J.A., Naderi, G.B., Dunning, B.E., Mangold, B.L., Mone, M.D., Russell, M.E., Weldon, S.C. & Hughes, T.E. (2002). 1-[2-[(5-Cyanopyridin-2-yl)amino]ethylamino]acetyl-2-(S)-pyrrolidinecarbon nitrile: a potent, selective, and orally bioavailable dipeptidyl peptidase IV inhibitor with antihyperglycemic properties. J. Med. Chem. 45, 2362-2365; Pospisilik, J.A., Stafford, S.G., Demuth, H.U., McIntosh, C.H. & Pederson, R.A. (2002). Long-term treatment with dipeptidyl peptidase IV inhibitor improves hepatic and peripheral insulin sensitivity in the VDF zucker rat: a euglycemic-hyperinsulinemic clamp study. Diabetes 51, 2677-2683).

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Therefore, the present invention provides a solution to the problem of identifying and/or designing inhibitors of DPP-IV activity by providing crystals of the extracellular domain of DPP-IV and their crystal structure information, methods of preparing such

crystals, and methods of identifying and/or designing inhibitors of DPP-IV with these crystals by structure based drug design.

The present invention relates to crystal structure information obtained from crystalline preparations of the dipeptidyl-peptidase DPP-IV, to methods of preparing such crystals, and to their use for the identification and/or design of inhibitors of DPP-IV activity. A further subject matter of the invention are methods for the identification and/or design of inhibitor compounds of DPP-IV activity, the inhibitor compounds of DPP-IV activity identified by these methods and their use in pharmaceutical compositions for the treatment and/or prevention of diseases comprising diabetes types I and II, obesity and cancer.

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Figure 1. Sequence alignment of DPP-IV and POP: Amino acid sequence alignment of DPP-IV from human (hDPP-IV) and rat (rDPP-IV, only different residues are shown). The alignment of POP from pork was performed using structural superposition for the α/β -hydrolase domain only, because of a lack of structural homology for the β -propeller domain. The top line gives additional information about the secondary structure of DPP-IV (yellow arrows and red bars), the glycosylation sites with visible electron density (Y), the potential glycosylation sites (marked in red), the disulphide bonds (green lines between cysteins that are involved) and an arrow that indicates the start of the cloned ectodomain. Sequences are highlighted light gray for the transmembrane part, gray for the part of the β -propeller involved in dimerization, green for residues involved in adenosine deaminase binding, blue for the tyrosine that is involved in the stabilization of the oxyanion of the catalytic intermediate and pink for the catalytic residues.

Figure 2. Overall Structure of DPP-IV: Ribbon diagram of DPP-IV viewed perpendicular to the two-fold axis. The domains are colored dark green and light green for the α/β hydrolase and β-propeller domains of subunit A and dark/light blue for the other subunit, respectively. The overall dimension of the molecule is about 125 x 80 x 60 Å³. The active site is highlighted by the catalytic residues in ball and stick representation as well as residues that are identified by mutagenesis data to be important for ADA binding. The proposed location at the cell surface is shown by the schematic drawing of the membrane. This figure was prepared using Molscript (Kraulis, P.J. (1991). MOLSCRIPT: A program to produce both detailed and schematic plots of protein structures. J. Applied Crystallogr. 24, 946-950) and rendered with Raster3D (Merrit, E.A. & Bacon, D.J. (1997). Raster3D: photorealistic molecular graphics. Methods Enzymol. 277, 505-524).

Figure 3. Ribbon drawing of the β -propeller domains of DPP-IV and POP: A: DPP-IV has 8 repeats of a structural motif that consists of four antiparallel β -strands or blades (blades are numbered 1 to 8). Additional secondary structural elements are colored magenta: An antiparallel β -sheet (β 2/2a and β 2/2b in Figure 1) that is an extension of blade 2 with Arg125 at the tip of the turn that is involved in the substrate binding. An α -helix (α 2* in Figure 1) with the C-terminal glutamate rich loop that contributes to substrate recognition and specificity (Glu204/205/206). The antiparallel β -sheet that forms a main part of the dimer interface (β 1* and β 2* in Figure 1). The latter structural elements are extensions of the blade 4.

B: β-propeller domain of DPP-IV rotated 90°
C: POP has 7 blades and no notable deviations from the β-propeller structure. The blades are numbered 1 to 7.

Figure 4. Access to the active site: Schematic view on the subunit of DPP-IV with the active site surface coloured according to the atom types. The substrate Diprotin A is shown with white carbons indicating the substrate binding site. Arrows illustrate that the substrate may enter the active site at the well accessible and open active site cleft and the dipeptidic product of the catalytic reaction may leave the active site cavity via the more narrow tunnel that is formed by the β -propeller.

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Figure 5. Active site of DPP-IV with Diprotin A (Ile-Pro-Ile): The substrate Diprotin A is trapped as tetrahedral intermediate covalently bound to the active site Ser630. Dashed lines indicate hydrogen bonds. Bonds are dark blue for the protein and light blue for the ligand as well as the active site Ser630. Drawn with MOLOC (Gerber, P.R. (1992). Peptide mechanics: a force field for peptides and proteins working with entire residues as small unites. *Biopolymers* 32, 1003-1017). The insert shows the omit electron density (ligand and Ser630 were omitted from the calculations) contoured at 2.5 σ (green) and 4 σ (yellow).

The present invention relates to crystals of mammalian DPP-IV, with or without a ligand bound in the active site, where the crystals are of sufficient quality and size to allow for the determination of the three-dimensional X-ray diffraction at atomic resolution. The invention also relates to methods for producing and crystallizing the mammalian DPP-IV. The crystals of mammalian DPP-IV, as well as information derived from their crystal structures can be used to analyze and modify mammalian DPP-IV activity as well as to identify compounds that interact with DPP-IV.

In one aspect the present invention provides a crystal of the extracellular domain of mammalian DPP-IV, preferably having the orthorhombic space group symmetry $P2_12_12_1$ and one homodimer of DPP-IV in the asymmetric unit. Preferably, the crystal includes a unit cell having dimensions a, b, and c; wherein a is from 63Å to 67Å, b is from 66 Å to 70 Å, and c is from 416 Å to 424 Å; and $\alpha = \beta = \gamma = 90^{\circ}$. Preferably, the crystal includes atoms arranged in a spatial relationship represented by the atomic structure coordinates listed in Table 4. Preferably, the crystal includes DPP-IV comprising the amino acid sequence from Gly31 to Pro766 of the native protein as well as shorter variants thereof comprising all amino acids necessary for forming the active site. Preferably, the crystal includes DPP-IV as set forth in SEQ ID NO:2 as well as shorter variants thereof comprising all amino acids necessary for forming the active site.

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The crystals of the invention include apo crystals and co-crystals. The apo crystals of the invention refer to crystals of mammalian DPP-IV formed without a bound active site or allosteric ligand. The co-crystals generally comprise DPP-IV with a ligand bound to the active site or to an allosteric site. The "active site" refers in general to the site where the enzymatic reaction catalyzed by the enzyme takes place. An active site ligand refers to any compound which specifically binds to the active site of a mammalian DPP-IV.

Preferably, the co-crystal of the present invention is characterized as having an orthorhombic space group of P2₁2₁2₁ (space group No. 19) and one homodimer of DPP-IV in the asymmetric unit.

More preferably, the co-crystal has unit cell dimensions of a is from 63 Å to 67Å, b is from 66 Å to 70 Å, and c is from 416 Å to 424 Å.; and $\alpha = \beta = \gamma = 90^{\circ}$ and a $P2_12_12_1$ symmetry.

The co-crystals of the invention generally comprise a crystalline DPP-IV polypeptide in association with one or more compounds at an active or allosteric binding site of the polypeptide. The association may be covalent or non-covalent.

The DPP-IV (dipeptidyl-peptidase, DPP-IV; T-cell activation antigen CD26 or adenosine binding protein) of the present invention may be a mammalian DPP-IV. Preferably, the DPP-IV of the present invention is a human DPP-IV. More preferably, the DPP-IV of the present invention is the extracellular domain of DPP-IV. Even more preferred is the extracellular domain of DPP-IV which is soluble. Most preferably, the human DPP-IV comprises the amino acid sequence from Gly31 to Pro766 of the native

protein as well as shorter variants thereof comprising all amino acids necessary for forming the active site. Preferably, DPP-IV comprises the amino acid sequence as set forth in SEQ. ID NO:2 as well as shorter variants thereof comprising all amino acids necessary for forming the active site.

It is to be understood that the crystals of DPP-IV of the invention are not limited to naturally occurring or native DPP-IV. Indeed, the crystals of the invention include mutants of the native DPP-IV. Mutants of native DPP-IV are obtained by replacing at least one amino acid residue in a native DPP-IV domain with a different amino acid residue, or by adding or deleting amino acid residues within the native polypeptide or at the N- or C- terminus of the native polypeptide, and have substantially the same three-dimensional structure as the native DPP-IV from which the mutant is derived.

By having substantially the same three-dimensional structure is meant having a set of atomic structure coordinates from an apo- or co-crystal that have a root mean square deviation of less than or equal to about 1.5 Å when superimposed with the atomic structure coordinates of the native DPP-IV when at least 50% of the alpha carbon atoms of DPP-IV are included in the superposition.

In some instances, it may be particularly advantageous or convenient to substitute, delete and/or add amino acid residues to a native DPP-IV domain in order to provide convenient cloning sites in cDNA encoding the polypeptide, to aid in purification of the polypeptide, etc. Such substitutions, deletions and/or additions which do not substantially alter the three dimensional structure of the native DPP-IV will be apparent to those having skills in the art.

It should be noted that the mutants contemplated herein need not exhibit DPP-IV activity. Indeed, amino acid substitutions, additions or deletions that interfere with the peptidase activity of the DPP-IV but which do not significantly alter the three-dimensional structure of the domain are specifically contemplated by the invention. Such crystalline polypeptides, or the atomic structure coordinates obtained therefrom, can be used to identify compounds that bind to the native domain. These compounds may affect the activity or the native domain.

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The derivative crystals of the invention generally comprise a crystalline DPP-IV polypeptide in covalent association with one or more heavy metal atoms. The polypeptide may correspond to a native or a mutated DPP-IV. Heavy metal atoms useful for providing derivative crystals include, by way of example and not limitation, gold and mercury. Alternatively, derivative crystals can be formed from proteins which have heavy atoms

incorporated into one or more amino acids, such as seleno-methionine substitutions for methionine.

Therefore, in a preferred embodiment of the present invention the co-crystal is a co-crystal of the extracellular domain of mammalian DPP-IV and HgCl₂.

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The native and mutated DPP-IV polypeptides described herein may be isolated from natural sources or produced by methods well known to those skilled in the art of molecular biology. Expression vectors to be used may contain a native or mutated DPP-IV polypeptide coding sequence and appropriate transcriptional and/or translational control signals. These methods include *in vitro* recombinant DNA techniques, synthetic techniques and *in vivo* recombination/genetic recombination. See, for example, the techniques described in Maniatis et al., 1989, *Molecular Cloning: A Laboratory Manual*, Cold Spring Harbor Laboratory, NY; and Ausubel et al., 1989, *Current Protocols in Molecular Biology*, Greene Publishing Associates and Wiley Interscience, NY.

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A variety of host-expression vector systems may be utilized to express the DPP-IV coding sequence. These include but are not limited to microorganisms such as bacteria transformed with recombinant bacteriophage DNA, plasmid DNA or cosmid DNA expression vectors containing the DPP-IV coding sequence; yeast transformed with recombinant yeast expression vectors containing the DPP-IV coding sequence; insect cell systems infected with recombinant virus expression vectors (e.g. baculovirus) containing the DPP-IV coding sequence; plant cell systems infected with recombinant virus expression vectors (e.g., cauliflower mosaic virus, CaMV; tobacco mosiac virus, TMV) or transformed with recombinant plasmid expression vectors (e.g., Ti plasmid) containing the DPP-IV coding sequence; or animal cell systems. The expression elements of these systems vary in their strength and specificities. Depending on the host/vector system utilized, any of a number of suitable transcription and translation elements, including constitutive and inducible promoters such as pL of bacteriophage µ, plac, ptrp, ptac (ptrplac hybrid promoter) and the like may be used; when cloning in insect cell systems, promoters such as the baculovirus polyhedrin promoter may be used; when cloning in plant cell systems, promoters derived from the genome of plant cells (e.g., heat shock promoters; the promoter for the small subunit of RUBISCO; the promoter for the chlorophyll a/b binding protein) or from plant viruses (e.g., the 35 S RNA promoter of CaMV; the coat protein promoter of TMV) may be used; when cloning in mammalian cell systems, promoters derived from the genome of mammalian cells (e.g., metallothionein

promoter) or from mammalian viruses (e.g., the adenovirus late promoter; the vaccinia virus 7.5K promoter) may be used; when generating cell lines that contain multiple copies of the DPP-IV coding sequence, SV40-, BPV- and EBV-based vectors may be used with an appropriate selectable marker.

In a preferred embodiment of the present invention, an isolated nucleic acid sequence encoding the soluble extracellular domain of DPP-IV comprising the nucleotide sequence of SEQ ID NO:1 is provided.

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Additionally, an expression vector containing an isolated nucleic acid sequence encoding the soluble extracellular domain of DPP-IV comprising the nucleotide sequence of SEQ ID NO:1 is provided. Preferably, the expression vector for the expression of proteins in P. pastoris which are to be secreted. Furthermore, a host cell transformed with the said expression vector is provided. Preferably, the host cell is *Pichia pastoris*.

A further aspect of the present invention relates to a method of producing the soluble extracellular domain of DPP-IV comprising culturing the host cell with the said expression vector under conditions permitting the expression of the soluble extracellular domain of DPP-IV by the host cell. Preferably, the host cell is P. pastoris. The present invention also provides the soluble extracellular domain of DPP-IV produced by this method.

Furthermore, the present invention relates to a polypeptide comprising the soluble extracellular domain of DPP-IV as set forth in SEQ ID NO:2.

The apo-, derivative and co-crystals of the invention can be obtained by techniques well-known in the art of protein crystallography, including batch, liquid bridge, dialysis, vapor diffusion and hanging drop methods (see e.g. McPherson, 1982, *Preparation and Analysis of Protein Crystals*, John Wiley, NY; McPherson, 1990, *Eur. J. Biochem.* 189:1-23; Webber, 1991, *Adv. Protein Chem.* 41:1-36; Crystallization of Nucleic Acids and Proteins, Edited by Arnaud Ducruix and Richard Giege, Oxford University Press; Protein Crystallization Techniques, Strategies, and Tips, Edited by Terese Bergfors, International University Line, 1999). Generally, the apo- or co-crystals of the invention are grown by placing a substantially pure DPP-IV polypeptide in an aqueous buffer containing a precipitant at a concentration just below that necessary to precipitate the protein. Water is then removed from the solution by controlled evaporation to produce crystallizing conditions, which are maintained until crystal growth ceases.

Preferably, the crystals are produced by a method for crystallizing mammalian DPP-IV, the method comprising (a) providing a buffered, aqueous solution of pH 7 to 8.5 with a concentration of 7 mg/ml to 22 mg/ml of the extracellular domain of mammalian DPP-IV; and (b) growing crystals by vapor diffusion using a buffered reservoir solution with between 10% and 30% PEG, between 10% and 20% glycerol, wherein PEG has an average molecular weight between 1000 and 20000. More preferably, the extracellular domain of mammalian DPP-IV of step (a) of the method is produced in the yeast *Pichia pastoris* (*P. pastoris*) and then deglycosylated. For deglycosylation, different enzymes may be used comprising Endoglycosidase F or PNGase.

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Preferably, co-crystals are produced by a method for co-crystallizing mammalian DPP-IV and an active site ligand, the method comprising (a) providing a buffered, aqueous solution of pH 7 to 8.5 with a concentration of 7 mg/ml to 22 mg/ml of the extracellular domain of mammalian DPP-IV; (b) adding a molar excess of the active site ligand to the aqueous solution of mammalian DPP-IV; (c) growing crystals by vapor diffusion using a buffered reservoir solution with between 10% and 30% PEG, between 10% and 20% glycerol, wherein PEG has an average molecular weight between 1000 and 20000. More preferably, the extracellular domain of mammalian DPP-IV of step (a) of the method is produced in P. pastoris and then deglycosylated.

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A further aspect of the present invention relates to a crystal produced by the methods for crystallizing or co-crystallizing DPP-IV of the present invention.

Crystals may be frozen prior to data collection.

The mosaic spread of the frozen crystals could sometimes be reduced by annealing, wherein the stream of cold nitrogen gas is briefly blocked, allowing the frozen crystal to thaw momentarily before re-freezing in the nitrogen gas stream.

Diffraction data typically extending to 2.7 Å was collected from the frozen crystals at the synchrotron beamline x06 at the Swiss light source (SLS), Villigen Switzerland. Under optimum conditions, data extending to 2.1 Å was recorded. Preferably, the data is collected at a resolution of 3.5 Å to 2.1 Å or better. More preferably, the data is collected at a resolution of 2.7 Å to 2.1 Å or better.

Derivative crystals of the invention can be obtained by soaking apo or co-crystals in mother liquor containing salts of heavy metal atoms, according to procedures known to those of skill in the art of X-ray crystallography.

Co-crystals of the invention can be obtained by soaking an apo crystal in mother liquor containing a ligand that binds to the active site, or can be obtained by co-crystallizing the DPP-IV polypeptide in the presence of one or more ligands that bind to the active site or to an allosteric site. Preferably, co-crystals are formed with an active site DPP-IV ligand which is slowly hydrolysable and forms a covalent bond. One example for such an active site ligand is Diprotin A.

In a further embodiment of the present invention a method for determining the three-dimensional structure of a crystallized extracellular domain of mammalian DPP-IV to a resolution of 3.5 Å to 2.1 Å or better is provided, the method comprising (a) crystallizing an extracellular domain of mammalian DPP-IV; and (b) analyzing the extracellular domain of mammalian DPP-IV by X-ray diffraction to determine the three-dimensional structure of the crystallized extracellular domain of mammalian DPP-IV, whereby the three-dimensional structure of a crystallized extracellular domain of mammalian DPP-IV is determined to a resolution of about 3.5 Å to 2.1 Å or better.

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The present invention further relates to a machine-readable data storage medium comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, displays a graphical three-dimensional representation of a molecule or molecular complex comprising at least a portion of the extracellular domain of mammalian DPP-IV comprising the amino acids of SEQ ID NO:2, the extracellular domain comprising the ligand binding active site being defined by a set of points having a root mean square deviation of less than about 1.5Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 4.

The crystals of the invention, and particularly the atomic structure coordinates obtained therefrom, have a wide variety of uses. For example, the crystals and structure coordinates described herein are particularly useful for identifying compounds that interact with DPP-IV as an approach towards developing new therapeutic agents. Pharmaceutical compositions of said compounds can be developed, and said compounds can be used for the manufacture of a medicament comprising said compound for the treatment of IGT, type I and type II diabetes, obesity and cancer.

Therefore, the present invention also relates to the use of a crystal or a co-crystal of the invention for the identification and/or design of inhibitors of DPP-IV activity.

Moreover, the present invention relates to a method for identifying a compound that interacts with DPP-IV, comprising the steps of

- (a) generating a three-dimensional model of DPP-IV using the structure coordinates listed in Table 4, a root mean square deviation from the backbone atoms of said amino acids of less than 1.5Å; and
- (b) employing said three-dimensional model to design or select a compound that interacts with DPP-IV.

In another aspect, the method further comprises the steps of

(c) obtaining the identified compound; and

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- (d) contacting the obtained compound with DPP-IV in order to determine the effect the compound has on DPP-IV activity.
- The compound in these methods may be a compound that interacts with the active site of DPP-IV or may be a compound that interacts with an allosteric site of DPP-IV. Preferred are compounds which interact with the active site of DPP-IV. Even more preferred are compounds, which show an inhibitory effect on DPP-IV activity in step (d) of the methods of the present invention.
- In a further aspect of the present invention the method for identifying a compound that interacts with DPP-IV is a computer-assisted method. Preferably, determining whether the compound is expected to bind to or interfere with the molecule or molecular complex includes performing a fitting operation between the compound and a binding site or substrate binding surface of the molecule or molecular complex, followed by computationally analyzing the results of the fitting operation to quantify the association between, or the interference with, the compound and the binding site. Optionally, the method further includes screening a library of compound. Optionally, the method further includes supplying or synthesizing the compound, then assaying the compound to determine whether it interacts with and has an effect on mammalian DPP-IV activity.
- The present invention also relates to the compounds identified by the said methods for identifying a compound that interacts with DPP-IV.

The structure coordinates described herein can be used as phasing models in determining the crystal structures of additional native or mutated DPP-IV, as well as the structures of co-crystals of such DPP-IV with active site inhibitors or activators bound. The structure coordinates, as well as models of the three-dimensional structures obtained therefrom, can also be used to aid the elucidation of solution-based structures of native or mutated DPP-IVs, such as those obtained via NMR. Thus, the crystals and atomic structure coordinates of the invention provide a convenient means for elucidating the structures and functions of DPP-IV or other prolyl oligopeptidases.

For purposes of clarity and discussion, the crystals of the invention will be described by reference to specific DPP-IV exemplary apo crystals and co-crystals. Those skilled in the art will appreciate that the principles described herein are generally applicable to crystals of any mammalian DPP-IV, including, but not limited to DPP-IV.

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Increased levels of glucagon like peptide 1 (GLP1) are beneficial for the decrease of plasma glucose in humans. The finding that DPP-IV is responsible for more than 95% of the degradation of GLP-1 led to an elevated interest in inhibition of this enzyme for the treatment of diabetes type II. Experiments in rats and humans have provided evidence that specific DPP-IV inhibition increased C_{max} , $T_{1/2}$ and total circulating GLP-1 and decreased plasma glucose. It has been demonstrated that patients with impaired glucose-tolerance (IGT), type-II diabetes and with a secondary failure to respond to sulfonylurea treatment benefit from increased levels of GLP1 peptides. In addition GLP-1 is effective in type-I diabetic patients due to its glucagono-static effect. More recent investigations show a delay of gastric emptying that could have beneficial effects on satiety and might be relevant for the treatment of obesity. Protection of functional GLP-1 by inhibition of DPP-IV and concomitant activation of the GLP-1 receptor might therefore have a synergistic potential in anti-diabetic drug research (Holst, J.J. & Deacon, C.F. (1998). Inhibition of the activity of dipeptidyl-peptidase IV as a treatment for type 2 diabetes. Diabetes 47, 1663-1670). Selective and orally available small molecule inhibitors of DPP-IV have been discovered and are now in clinical trials.

Therefore, in a further aspect of the present invention a pharmaceutical composition comprising the compound identified by the methods of the present invention as having an effect on DPP-IV activity, or pharmaceutically acceptable salts thereof, and a pharmaceutically acceptable carrier is provided.

The phrase "pharmaceutically acceptable" is employed herein to refer to those compounds, materials, compositions, and/or dosage forms which are, within the scope of

sound medical judgment, suitable for use in contact with the tissues of human beings and animals without excessive toxicity, irritation, allergic response, or other problem or complication, commensurate with a reasonable benefit/risk ratio.

As used herein, "pharmaceutically acceptable salts" refer to derivatives of the disclosed compounds wherein the parent compound is modified by making acid or base salts thereof. Examples of pharmaceutically acceptable salts include, but are not limited to, mineral or organic acid salts of basic residues such as amines; alkali or organic salts of acidic residues such as carboxylic acids; and the like. The pharmaceutically acceptable salts include the conventional non-toxic salts or the quaternary ammonium salts of the parent compound formed, for example, from non-toxic inorganic or organic acids. For example, such conventional non-toxic salts include those derived from inorganic acids such as hydrochloric, hydrobromic, sulfuric, sulfamic, phosphoric, nitric and the like; and the salts prepared from organic acids such as acetic, propionic, succinic, glycolic, stearic, lactic, malic, tartaric, citric, ascorbic, pamoic, maleic, hydroxymaleic, phenylacetic, glutamic, benzoic, salicylic, sulfanilic, 2-acetoxybenzoic, fumaric, benzenesulfonic, toluenesulfonic, methanesulfonic, ethane disulfonic, oxalic, isethionic, and the like.

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The pharmaceutically acceptable salts of the present invention can be synthesized from the parent compound which contains a basic or acidic moiety by conventional chemical methods. Generally, such salts can be prepared by reacting the free acid or base forms of these compounds with a stoichiometric amount of the appropriate base or acid in water or in an organic solvent, or in a mixture of the two; generally, nonaqueous media like ether, ethyl acetate, ethanol, isopropanol, or acetonitrile are preferred. Lists of suitable salts are found in Remington's Pharmaceutical Sciences, 17th ed., Mack Publishing Company, Easton, PA, 1985, p. 1418, the disclosure of which is hereby incorporated by reference.

"Stable compound" and "stable structure" are meant to indicate a compound that is sufficiently robust to survive isolation to a useful degree of purity from a reaction mixture, and formulation into an efficacious therapeutic agent.

Furthermore, a compound identified by the methods of the present invention as having an effect on DPP-IV activity for use as a therapeutic active substance, in particular for the treatment of diabetes type I, diabetes type II, IGT, obesity and cancer, is provided.

A further aspect of the present invention relates to the use of a compound identified by the methods of the present invention as having an effect on DPP-IV activity for the manufacture of a medicament for the treatment of diabetes type-I, diabetes type-II, IG, obesity, and cancer. Having now generally described this invention, the same will become better understood by reference to the specific examples, which are included herein for purpose of illustration only and are not intended to be limiting unless otherwise specified, in connection with the following figures.

Examples

Commercially available reagents referred to in the examples were used according to manufacturer's instructions unless otherwise indicated.

Example 1

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5 DNA manipulation and sequence analysis

Preparation of DNA probes, digestion with restriction endonucleases, DNA ligation and transformation of E.coli strains were performed as described (Sambrook, J., Fritsch, E.F. & Maniatis, T. (1989). *Molecular Cloning: A Laboratory Manual*. Cold Spring Harbor Laboratory Press: Cold Spring Harbor, NY.). For DNA sequencing, the ABI PRISM BigDye Terminator Cycle Sequencing Ready Reaction Kit and ABI PRISM 310 Genetic analyzer were used. PCR were performed in the T3 Thermocycler (Whatman Biometra), using the Pfu polymerase (Stratagene).

Production and Purification of recombinant human sDPP-IV in P. pastoris

The ectodomain of DPP-IV, residues 31-766 (sDPP-IV), was amplified by PCR using a cDNA and the oligonucleotides 5'-TGCTGGAATTCGGCACAGATGATGCTAC-3' (with an EcoRI site in bold) and 5'-GCA TGG TAC CTT GAG GTG CTA AG -3' (with a KpnI site in bold). Using the two new restriction sites, the amplified DNA fragment (SEQ ID NO:1) was cloned into pPICZα-A vector (Invitrogen) to create a fusion with the α-mating factor signal sequence for the secretion of the protein. The use of the EcoRI restriction site added the amino acids glutamine and phenylalanine to the N-terminus of sDPP-IV. The sequence was confirmed by sequencing. pPICZα-sDPP-IV was linearized with SacI, transformed by electroporation in P. pastoris strain GS115 and the phenotype of the colonies obtained was checked as recommended by the distributor Invitrogen.

Eight transformants with phenotype MutS were screened for the expression of DPP-IV. Colonies were grown at 30°C in YPD medium (1% yeast extract, 2% peptone, 2% glucose) with zeocin (100 μg/ml) to an OD₆₀₀ of 8-10. Cells were collected by centrifugation and resuspended in YP medium plus 2% methanol. The same amount of methanol was added every 24 h. After 48 h the medium of each clone was tested for activity (see below). sDPP-IV was then produced in a large scale culture using the transformed cell line with the highest activity per volume as described (Dale, G.E., D'Arcy, B., Yuvaniyama, C., Wipf, B., Oefner, C. & D'Arcy, A. (2000). Purification and crystallization of the

extracellular domain of human neutral endopeptidase (neprilysin) expressed in Pichia pastoris. Acta Crystallogr. D 56, 894-897).

Ten liters of the collected sDPP-IV supernatant of the selected transformed P. pastoris cell line was filtered and concentrated to 180 ml by crossflow ultrafiltration (skannette) using a 30 kDA filtration module (AGT Technology corporation). The concentrate was passed over a Sephacryl 200 XK 50/100 size exclusion column (5 x 95 cm, Pharmacia) equilibrated with 50 mM Tris-HCl pH 7.8 and 100 mM NaCl (S-buffer). Collected fractions were screened on SDS-PAGE and for activity. Fractions containing sDPP-IV were dialysed against 50 mM Tris-HCl pH 7.9. The protein solution was loaded on a Fractogel-TMAE column (2.6 x 13 cm, Merck) equilibrated with 50 mM Tris-HCl pH 7.9, washed with two column volumes of the same buffer and eluted with 500 ml of a linear gradient from 0 to 200 mM NaCl. Fractions containing sDPP-IV were dialysed against 20 mM sodium acetat pH 4.8. The protein solution was loaded on a Fractogel-COO column (1 x 12 cm, Merck) equilibrated with the same buffer and washed with two column volumes of this buffer. Bound proteins were eluted with 200 ml of a linear gradient from 50 to 500 M NaCl. The elution profile showed a major peak at 250 mM NaCl. Preparation of enzymatically deglycosylated sDPP-IV (sDPPIV_{deglycos}) was carried out prior to loading on the last gelfiltration column. 0.1% EndoF1-GST was added to the pooled fractions of DPP-IV and incubated for 20 h at 21°C. The concentrated protein solution was loaded on a Biosec size exclusion column (1.6 x 60 cm, Merck), that was equilibrated with S-buffer. Fractions were analyzed by SDS-PAGE, showing a purity > 95%. N-terminal sequencing showed that the protein was efficiently processed by the STE13 signal peptidase which cleaves off the α-mating factor. Preparation of the sDPPIV_{deglycos}:ADA-complex was performed by addition of a two times excess of ADA (Sigma Type IV, from calf intestinal Mucosa) and purification using a Biosec-size exclusion column.

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The soluble extracellular domain of human dipeptidyl peptidase IV (sDPP-IV; residues 31-766) was expressed in the yeast Pichia pastoris. The protein was secreted at the low level of 1 mg/l as estimated from the total activity. As a first purification step the concentrated protein was passed through a size-exclusion column which removed the main fraction of contaminating peptides from the yeast-peptone medium. Sequential chromatography on anion- and cation-exchanger and a second size exclusion chromatography were used to get protein of 95% purity as judged by SDS-PAGE. The yield of pure protein was 0.3 mg/l growth medium. The purified protein shows essentially identical kinetic parameters and inhibition constants for known inhibitors of DPP-IV to those reported for the enzyme purified from human serum (Tables 1 and 2).

Analytical methods

Purification of sDPP-IV was followed by electrophoresis on 10-20% Tricine SDS polyacrylamide gradient gels (Lämmli, U.K. (1970). Cleavage of structural proteins during assembly of the head of bacteriophage T4. Nature 227, 680-685). Protein concentrations were determined according to Bradford (Bradford, M.M. (1976). A rapid and sensitive method for the quantitation of microgram quantities of protein utilizing the principle of protein-dye binding. Anal. Biochem. 72, 248-254) or for pure protein by absorption spectroscopy using the calculated molecular extinction coefficient at 280 nm of 193'920 M ¹cm⁻¹ (A₂₈₀^{0.1%} = 2.27cm²/mg; Pace, C.N., Vajdos, F., Fee, L., Grimsley, G. & Gray, T. (1995). How to measure and predict the molar absorption coefficient of a protein. Protein Sci 4, 2411-2423). Analytical gel filtration chromatography was performed on a Superdex 200 12 HR 10/30 column (Pharmacia) equilibrated with S-buffer. The eluate was monitored with a miniDAWN multi-angle laser light scattering detector (Wyatt) and a refractive index-detector (Shodex), which allows the determination of the molecular weight and dispersity over the elution peak (Wyatt, P.J. (1993). Light scattering and the absolute characterisation of macromolecules. Analytica Chimica Acta 272, 1-40). Sedimentation equilibrium runs in a Beckman analytical ultracentrifuge (model Optima XL A) were performed at 20°C and 9000 rpm sDPP-IV_{deglycos} and at 7000 rpm for sDPP-IV_{deglycos}:ADA-complex. The initial protein concentrations were 0.22 to 0.25 mg/ml in Sbuffer. The absorption was followed at 280 nm. Assumed partial specific volumes for sDPP-IV of 0.729 cm³/g and ADA of 0.735 cm³/g were used to determine the molecular masses.

Free sulfhydryl groups were determined according the procedure described by Ellman (Ellman, G.L. (1959). Tissue sulfhydryl groups. *Arch. Biochem. Biophys.* 82, 70-77) under denaturing conditions (0.3% SDS in 50 mM Tris pH 8.0).

Thermostability measurements

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The irreversible loss of activity after incubation at various temperatures was used as an operational criterion of the thermostability of sDPP-IV. Kinetics of irreversible heat inactivation were performed as described by Sterner et al. (Sterner, R., Kleemann, G.R., Szadkowski, H., Lustig, A., Hennig, M. & Kirschner, K. (1996). Phosphoribosyl anthranilate isomerase from Thermotoga maritima is an extremely stable and active homodimer. *Protein Sci.* 5, 2000-2008) with a final protein concentration of 20 µg/ml in 50 mM potassium phosphate buffer at pH 7.5, containing 100 mM NaCl. The residual activity was determined by recording the initial velocity at 25°C of the enzyme-catalyzed

reaction (see below) and the averaged values obtained were plotted against the incubation temperature.

Biacore

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DPP-IV was immobilized on a CM5 surface plasmon resonance sensor (Biacore) using standard amide coupling chemistry. The organic adlayer on this sensor type consists of carboxymethylated dextran (MW =100 kDA). After activation of the carboxylic acid groups using carbodiimide/N-hydroxysuccinimide solutions, the surface was contacted with a DPP-IV solution (80 μl) containing ≈ 100 μg/ml protein in acetate buffer (10 mM, pH 4.5). The amount immobilized corresponded to a sensor response of roughly 10 000 RU. The surfaces of two flow cells were modified with protein. To suppress baseline drift – possibly due to slow dimer dissociation – the protein of one cell was cross-linked by short contact with carbodiimide/N-hydroxysuccinimide solution. This treatment did not influence the protein activity since binding constants determined with cross - linked protein were similar to those determined with non-cross-linked protein. Hepes buffer (0.01 M Hepes, pH 7.4, 0.15 M NaCl, 3 mM EDTA, 0.005% polysorbate 20 (v/v)) was used as the running buffer. Diprotin-A was disolved directly in this buffer. NVP-DPP728 was first dissolved in pure DMSO and then diluted into running buffer. The final inhibitor solution contained less than 0.1% DMSO. Binding experiments were carried out by contacting the immobilized protein surfaces with inhibitor solutions of varying concentrations at a flow rate of 10 µl/min or 30 µl/min. After each contact with inhibitor, the protein surfaces were regenerated by extensively washing with running buffer.

Activity assay

The activity assay is based on the increase of fluorescence of products compared to the substrate Ala-Pro-7-amido-4-trifluoromethylcoumarin (Calbiochem, Smith, R.E., Reynolds, C.J. & Elder, E.A. (1992). The evolution of proteinase substrates with special reference to dipeptidylpeptidase IV. *Histochem. J.* 24, 637-647). A 20 mM stock solution in 10 % DMF is stored at -20° C until use. Purification was followed by using a final substrate concentration of 50 μ M and for the determination of kinetic parameters it was varied between 1.5 μ M and 500 μ M in the assay. DPP-IV activity assays were performed in 96 well plates in a total assay volume of 100 μ l. The assay buffer consists of S-Buffer containing 0.1 mg/ml BSA. Fluorescence is detected in a Luminescence Spectrometer LS 50B (Perkin Elmer) at an excitation wavelength of 400 nm and an emission wavelength of 505 nm. Initial rate constants are calculated by best fit linear regression.

Example 2

Crystallization and Structure determination

For crystallization trials, sDPP-IV_{deglycos} was concentrated to approximately 10 mg/ml. A reduced factorial screen was carried out using the vapour diffusion method. Crystals were obtained with 20-25% PEG 3350, 200 mM MgCl₂, Tris pH 8.5 and 15% glycerol. The crystals were flash-frozen in liquid nitrogen and exhibit the orthorhombic space group P2₁2₁2₁ with cell dimensions of about 65 Å, 68 Å and 420 Å and one dimer per asymmetric unit. They diffract to a maximum of 2.3 Å resolution using synchrotron radiation and show rather high mosaicity (0.5-1.2°). Addition of 1 mM Diprotin-A prior to crystallization led to crystals of the complex. The mercury derivative was produced by cocrystallization with 0.1 mM HgCl₂.

Data collection was performed using synchrotron radiation (Swiss light source, SLS Villigen, Switzerland and ID14, ESRF Grenoble, France) as well as in-house facilities (search for heavy atom derivatives, evaluation of crystal quality) and processed with DENZO (Otwinowski, Z. (1993). Oscillation data reduction program. In Proceedings of the CCP4 Study Weekend: Data Collection and Processing (Wawyey, L., Isaacs, N. & Bailey, S., eds.). pp. 56-62, SERC Daresbury Laboratory, UK). Details of the data collection statistics are given in Table 3. All programs used are part of the CCP4 (CCP4 (Collaborative Computational Project, Number 4) (1994). The CCP4 suite: programs for protein crystallography. Acta Crystallogr. D, 760-763) suite, except where indicated. The structure 20 was determined by multiwavelength anomalous dispersion (MAD) of the mercury derivative. One major mercury binding site per subunit (Cys 551, one of the two free SHgroups Cys301 and Cys551 that are located near the active site) was identified by inspection of the difference patterson maps calculated from the peak wavelength data and was subsequently refined using SHARP (De la Fortelle, E. & Bricogne, G. (1997). 25 Maximum likelihood heavy-atom parameter refinement for multiple isomorphus replacement and multiwavelength anomalous diffraction methods. Methods Enzymol. 276, 472-494). Location of the twofold non-crystallographic axis was performed using this mercury site and the program find2folds (Dunten, P. & Hennig, M. (2002). Locating noncrystallographic symmetry elements: The program Find2Folds. Acta Crystallogr. A58, 30 C76). Further analysis revealed another site per subunit (Cys301) with less occupancy and the site branched in two positions with about 2.4Å distance. Subsequently the phases were improved by application of twofold averaging combined with solvent flattening and histogram matching as implemented in DM. The initial electron density at 2.6 Å resolution was readily interpretable and about 90% of the polypeptide chain could be built. The 35 molecular model was refined against 2.3 Å data. Subsequent rounds of manual rebuilding and refinement with REFMAC (Murshudov, G.N., Vagin, A.A., Lebedev, A., Wilson, K.S.

& Dodson, E.J. (1999). Efficient anisotropic refinement of macromolecular structures using FFT. Acta Crystallogr. D 55, 247-255) led to a complete molecular structure of the polypeptide chain from residues Ser39 to Pro766. Details of the refined structures are reported in Table 3. Coordinates have been deposited in the Protein Data Bank PDB.

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Overall structure

The structure of human DPP-IV was solved by multiple anomalous dispersion (MAD) using a mercury derivative (see Table 3) and subsequently refined to an R-factor of 21.5 % at 2.1 Å resolution. The current model consists of all residues from Ser39 to Pro766 of the amino acid sequence of the expressed ectodomain of the protein.

A homodimer of DPP-IV is situated in the asymmetric unit (Figure 2). Dimerization is also observed in solution under various conditions and is required for activity. Each subunit is made of two domains, the catalytic domain with an α/β hydrolase fold containing the catalytic triad (Ser630, Asp708, His740) and a domain with an eight-bladed β -propeller fold, the β -propeller domain (Figure 2). The assignment of the secondary structure is given in Figures 1 and 2. The only other known crystal structure of this class of enzyme is prolyl-oligopeptidase (POP) determined by Fülop (Fülop, V., Bocskei, Z. & Polgar, L. (1998). Prolyl oligopeptidase: an unusual beta-propeller domain regulates proteolysis. *Cell* 94, 161-170; pdb entry 1qfm). POP also has an α/β -hydrolase and a β -propeller domain, but is monomeric and the β -propeller consists of seven repeats only (Figure 3C).

Catalytic Domain

The catalytic domain is built up of residues Gln508 to Pro766 and contains a central eight-stranded parallel β -sheet that is flanked by 12 helices known as α/β hydrolase fold. 21% sequence identity to POP indicates significant structural homology (Figure 1) and superposition of the central α -helix, carrying the catalytic Ser630 on its first turn, with the corresponding structure of POP gives an r.m.s deviation of 2.5 Ų for 238 residues. The catalytic domain is connected to the β -propeller by an N-terminal 15 residue linker, which is considerably shorter than the corresponding 76 residue region in POP. The residues lacking in DPP-IV are, however, replaced structurally and functionally by the C-terminal part of the catalytic domain of the second subunit of the dimer.

β-propeller domain

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The β -propeller domain is formed by the residues Lys56 to Asn497. The preceding N-terminal residues Ser39 to Leu55 form a loop structure with a small α -helix (α 1*, Figure 1) at the surface and in close proximity to the first residues of the catalytic domain. The β -propeller domain consists of an eight-fold repeat of a four-stranded antiparallel β -sheet motif (blade, Figure 3). The blades are in circular arrangement such that they form a solvent filled tunnel with a diameter of about 13 Å.

The β -propeller domain in DPP-IV does not form a joint β -sheet motif (described as molecular "velcro"; Fülop, V. & Jones, D.T. (1999). Beta propellers: structural rigidity and functional diversity. *Curr. Opin. Struct. Biol.* 9, 715-721; Paoli, M. (2001). Protein folds propelled by diversity. *Prog. Biophys. Mol. Biol.* 76, 103-130), but rather the blades show a regular arrangement (β 1/1 to β 7/4 or β 8/4) (Figure 3A) around the central axis forming a ring system that is not closed.

DPP-IV deviates from the regular β -propeller fold by additional secondary structural elements. An anti-parallel β -sheet is inserted in blade two between the strands one and two. The tip of the turn carries the residues Arg125 that forms a salt bridge with Glu205, that is situated at the C-terminal turn of an α -helix (residues Trp154 to Thr199), that is inserted between the first and second strands of blade 4. Arg125, Glu205 and the neighboring Glu204 form a significant part of the substrate binding site and are mainly responsible for the substrate specificity. An further anti-parallel β -sheet motif formed by residues Asp230 to Asn263 is inserted between the strands three and four of blade four (Figure 3B). This structural element forms a significant part of the dimer interface (see below).

Whereas the N-terminal β-sheet structure of the propeller has shorter strands and is somewhat tilted, the loop connecting the first and second β-sheet is longer, shows high temperature factors and may reduce the rigidity of the propeller architecture. The reduced stability of the circular domain structure at this position might be compensated by an extended hydrophobic cluster that consists of Ile63, Leu69, Ile76, Phe89, Leu90, Phe95, Phe98, Ile107, Ile114, Tyr135, Leu137 and Leu142, and a salt bridge between Arg61 and Asp104 and a hydrogen bond between the main chain NH of Arg61 and Tyr105. This distortion leads to a reduced height of the propeller at the positions between blade one and two (Figure 3B).

As no residues from the α/β hydrolase domain fill this up, a cleft between the two domains of the DPP-IV molecule is formed with a diameter of about 15 Å enabling access to the catalytic site (Figure 4). Therefore, we propose that DPP-IV has two independent

ways for the substrate and product to access and leave the active site, a cleft between the domains and the tunnel through the β -propeller. The open cleft may enable large peptides and partially folded proteins to access the active site. The more narrow tunnel could be an exit for the cleaved dipeptides (Figure 4). The crystal structure of POP shows that the cleft between the two domains does not exist and the tunnel through the β -propeller is more narrow with about 4 Å compared to about 13 Å for DPP-IV (Figure 3A and 3C). This structural difference is supported by the observation that DPP-IV can process much larger substrates compared to POP. Peptides with a length of up to about 80 residues appear to be good substrates of DPP-IV. Larger proteins may also be cleaved depending on their tertiary structure. POP is reported to hydrolyse substrates with a maximum size of about 30 residues, only (Polgar, L. (1992). Unusual secondary specificity of prolyl oligopeptidase and the different reactivities of its two forms toward charged substrates. *Biochemistry* 31, 7729-7735.). As the diameter of the β -propeller tunnel in POP is significantly smaller, it is conceivable that the structure of DPP-IV represents a more open and active enzyme.

The β-propeller motif has been found in several further proteins, but no or only low sequence homology could be demonstrated (Polgar, L. (1992). Unusual secondary specificity of prolyl oligopeptidase and the different reactivities of its two forms toward charged substrates. *Biochemistry* 31, 7729-7735.). A search of the PDB for homologous structures gave the best results for clathrin (7 blades, ter Haar, E., Musacchio, A., Harrison, S.C. & Kirchhausen, T. (1998). Atomic structure of clathrin: a beta propeller terminal domain joins an alpha zigzag linker. *Cell* 95, 563-573), methylamine dehydrogenase (7 blades, Chen, L., Doi, M., Durley, R.C., Chistoserdov, A.Y., Lidstrom, M.E., Davidson, V.L. & Mathews, F.S. (1998). Refined crystal structure of methylamine dehydrogenase from Paracoccus denitrificans at 1.75 Å resolution. *J. Mol. Biol.* 276, 131-149) and nitrite reductase (8 blades, Nurizzo, D., Cutruzzola, F., Arese, M., Bourgeois, D., Brunori, M., Cambillau, C. & Tegoni, M. (1998). Conformational changes occurring upon reduction and NO binding in nitrite reductase from Pseudomonas aeruginosa. *Biochemistry* 37, 13987-13996), but no DPP-IV related function can be expected.

Active site

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The catalytic triad (Ser630, Asp708, His740) is located in a large cavity at the interface of the two domains. Ser630 is found at the tip of a very sharp turn between β -strand 5 and helix C, called the nucleophile elbow, which is a characteristic of hydrolases of the α/β type (Ollis, D.L., Cheah, E., Cygler, M., Dijkstra, B., Frolow, F., Franken, S.M., Harel, M., Remington, S.J., Silman, I., Schrag, J. & et al. (1992). The alpha/beta hydrolase fold. *Protein Eng.* 5, 197-211). The serine hydroxy group is well exposed to solvent and

hydrogen bonded to the catalytic imidazole group of His740 on one side (2.6 Å) and accessible to the substrate on the other side. His740 is found in the middle of a loop between β -strand 8 and helix F. With a distance of 2.75 Å to Ne of the imidazole ring, one of the oxygen atoms of Asp708 is hydrogen bonded to His740 and completes the catalytic triad (Figure 5). The other oxygen atom of the carboxylate group of Asp708 is coordinated by two main chain NH-groups (Val711 and Asn710). Thus, the location and geometry of the triad are very similar to that found in other α/β hydrolases with the "handedness" opposite to the classical serine peptidases.

The negatively charged oxyanion of the tetrahedral intermediate is stabilized by the
main chain NH-group of Tyr631 and by the hydroxy group of Tyr547 (Figure 5).
Furthermore, the structure shows that the two Gly628 and Gly632 are important for the
formation of the sharp turn to bring the catalytic residue Ser630 in the correct position.
This is in accordance with mutagenesis studies on rat DPP-IV (Ogata, S., Misumi, Y.,
Tsuji, E., Takami, N., Oda, K. & Ikehara, Y. (1992). Identification of the active site residues
in dipeptidyl peptidase IV by affinity labeling and site-directed mutagenesis. *Biochemistry*31, 2582-2587) showing that the sequence Gly628-X-Ser630-Tyr631-Gly632 is essential for
DPP-IV activity.

Substrate binding

The substrate binding site of DPP-IV is indicated by the inhibitor Diprotin-A (Ile-Pro-Ile). It is a slowly hydrolysable substrate with k_{cat}/K_M a factor of 10 less than Ile-Pro-4-nitroanilides (Rahfeld, J., Schierhorn, M., Hartrodt, B., Neubert, K. & Heins, J. (1991). Are diprotin A (Ile-Pro-Ile) and diprotin B (Val-Pro-Leu) inhibitors or substrates of dipeptidyl peptidase IV? *Biochim. Biophys. Acta* 1076, 314-316). Inspection of the electron density map shows the ligand covalently bound to the active site Ser630 of the enzyme in both subunits. The N-terminal Ile (P2) and Pro residues (P1) are well defined and enable a detailed analysis of the interaction with the substrate binding site (according to the notation of Schechter; Schechter, I. & Berger, A. (1968). On the active site of proteases. 3. Mapping the active site of papain; specific peptide inhibitors of papain. *Biochem. Biophys. Res. Commun.* 32, 898-902). Less well defined electron density is found for the C-terminal Ile (P1'), but in subunit B the conformation of this part of the ligand could also be observed (Figure 5). The side chain Nε of the catalytic His740 is in hydrogen bonding distance to the NH-group of P1' (2.90 Å) and to the Oγ of the Ser630 side chain (2.74 Å).

DPP-IV hydrolyzes oligopeptides and proteins from the N-terminus, cleaving dipeptide units when the second residue is proline, hydroxyproline, dehydroproline,

pipecolic acid or alanine. In both subunits the proline in position P1 of Diprotin-A is in the trans-configuration and fits optimally into the pocket of the active site as expected (Fischer, G., Heins, J. & Barth, A. (1983). The conformation around the peptide bond between the P1- and P2-positions is important for catalytic activity of some proline-specific proteases. *Biochim. Biophys. Acta* 742, 452-462). The S1 pocket is formed by Val711, Val656, Tyr662, Tyr666, Tyr659 and Tyr631 which shape a well defined hydrophobic pocket that would be filled by proline much better than by alanine. Gly is also accepted, but with very low k_{cat}/K_M values (Brandt, W., Lehmann, T., Thondorf, I., Born, I., Schutkowski, M., Rahfeld, J.U., Neubert, K. & Barth, A. (1995). A model of the active site of dipeptidyl peptidase IV predicted by comparative molecular field analysis and molecular modelling simulations. *Int. J. Pept. Protein Res.* 46, 494-507). All other naturally ocurring amino acids residues cannot occupy position P1. Either the side chains are too bulky or hydrophilic. The side chains of the residues P2 and P1' point into the solvent and no interaction with the protein occurs. This explains the large diversity of amino acids accepted in substrates at these positions.

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Essential for substrate binding and catalysis is the N-terminus of the substrates, which has to be unprotected and protonated (Brandt, W., Ludwig, O., Thondorf, I. & Barth, A. (1996). A new mechanism in serine proteases catalysis exhibited by dipeptidyl peptidase IV (DP IV) - Results of PM3 semiempirical thermodynamic studies supported by experimental results. Eur. J. Biochem. 236, 109-114). The Diprotin-A complex shows that the terminal -NH₃⁺ -group is held very precisely in position by strong interactions with the carboxylates of Glu205 and Glu206 (Figure 5). A third glutamate, Glu204, stabilizes this substrate recognition site by an hydrogen bonding network with the backbone NH of Arg125, His126 and Ser127 as well as the hydroxy group of Ser127. Importance of the glutamate residues is confirmed by single point mutations that abolish DPP-IV activity (Abbott, C.A., McCaughan, G.W. & Gorrell, M.D. (1999). Two highly conserved glutamic acid residues in the predicted beta propeller domain of dipeptidyl peptidase IV are required for its enzyme activity. FEBS Lett. 458, 278-284). The double Glu-motif is located at the end of an helical segment (α 2* in Figure 1, see also Figure 3) that is highly conserved in the DPP IV-like gene family (Asp-Trp-X-Tyr-Glu-Glu-Glu-X). The helix represents a deviation from the regular β -sheet architecture of the β -propeller domain (Figures 1 and 3A). The superposition of the active sites of the exopeptidase DPP-IV complexed with Diprotin A and the endopeptidase POP complexed with an octapeptide (Fülöp, V., Szeltner, Z., Renner, V. & Polgar, L. (2001). Structures of prolyl oligopeptidase substrate/inhibitor complexes. Use of inhibitor binding for titration of the catalytic histidine residue. J. Biol. Chem. 276, 1262-1266) shows clear differences. The octapeptide substrate of POP coincides with the double Glu-motif in DPP-IV indicating that this additional structural element functions is very important for substrate selection. Thus, the

double Glu-motif is a recognition site for the N-terminus of substrates and restricts the cleavage to dipeptides and the S1 pocket provides an optimal binding to proline and alanine residues leading to a highly specific peptidase.

Mode of inhibition by Diprotin-A

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Inspection of the electron density of the bound inhibitor shows a covalent linkage to Ser630 and a sp³-configuration for the C-atom of the former carbonyl-group of the scissile peptide. Consequently, a tetrahedral intermediate is observed in the complex structure with the substrate Diprotin A (Figure 5) with the oxyanion stabilized by hydrogen bonds to the hydroxy group of the side chain of Tyr547 (2.80 Å) and the main chain amine of Tyr631 (3.38 Å). As much catalytic power of serine proteases derives from its preferential binding of this transition state, the tetrahedral intermediate is a well-defined but high energy state with a short lifetime and its accumulation must be a result of a kinetic barrier.

Inspection of the active site structure reveals several structural features that are special to Diprotin A and may lead to the competitive inhibition of this substrate. First, the two hydrophobic isoleucine side chains point into the same direction in proximity and, therefore, this hydrophobic interaction may stabilize the tripeptide in a unsuitable conformation for the progress of the reaction. Second, a large network of salt bridges and hydrogen bonds stabilize the complex. It involves the carboxyl groups of Glu205/206 that interact with the N-terminus of the tripeptide, but Glu205 makes another salt bridge to Arg125 and this in turn interacts with the C-terminal carboxyl group of the tripeptide (Figure 5). It is obvious that this interaction is only present in tripeptidic substrates and may stabilize the observed intermediate by protection of the leaving group.

25 Dimerization

The crystal structure as well as analytical ultracentrifugation indicate dimeric oligomerization for deglycosylated sDPP-IV with a molecular weight of 169 kDa and noncrystallographic twofold symmetry (Figure 2). Six percent or 1837 Å² of the total solvent accessible surface area of each subunit is buried in the dimer interface (program XSAE, Broger, C. personal communication). This interface is mainly build up by two extra β -strands (β 1* and β 2*) in the loop between the strands two and three of the fourth blade of the β -propeller domain (Figure 3A and 3B). Further interaction is provided by the α/β hydrolase domain with helix α E, β -strand β 8 and helix α F with mainly hydrophobic interactions. The active site is very close to this dimer interface (Figure 2) with His740

from the catalytic triad located in the loop connecting αF and $\beta 7$ (Figure 1). Consequently disruption of the dimer interface would also strongly affect the catalytic activity and dimerization is required for activity.

Stability of DPP-IV

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As a cell surface protein DPP-IV is extremely stable. Consequently the recombinant sDPP-IV shows a half life of 5 min at 71°C in irreversible heat inactivation experiments independent of the protein concentration and the degree of glycosylation indicating high thermal stability. In unfolding experiments (Lambeir, A.M., Diaz Pereira, J.F., Chacon, P., Vermeulen, G., Heremans, K., Devreese, B., Van Beeumen, J., De Meester, I. & Scharpe, S. (1997). A prediction of DPP IV/CD26 domain structure from a physico-chemical investigation of dipeptidyl peptidase IV (CD26) from human seminal plasma. *Biochim. Biophys. Acta* 1340, 215-2) with protein purified from human seminal plasma DPP-IV retained its native conformation up to 8 M Urea.

The crystal structure points to several factors that may contribute to this stability. Firstly, the structural organization as a dimer with an extended hydrophobic interface stabilizes the molecule as shown for several other proteins (Thoma, R., Hennig, M., Sterner, R. & Kirschner, K. (2000). Structure and function of mutationally generated monomers of dimeric phosphoribosylanthranilate isomerase from Thermotoga maritima. Structure Fold. Des. 8, 265-276). Secondly, we observe five disulphide bonds and two free sulfhydryl groups by SH titration experiments under denaturing conditions that are now confirmed by the X-ray structure. All disulphide bridges in the β-propeller connect different strands in blades or stabilize loops (Cys444/Cys447; Cys385/Cys394, Cys454/Cys472, Cys328/Cys339). One disulfide bond is observed in the α/β-hydrolase domain (Cys649/Cys762) and covalently links the C-terminal helix αF to the core of the α/β hydrolase domain.

Glycosylation

sDPP-IV overexpressed in P. pastoris shows a decreasing molecular weight over the elution peak in the analytical gelfiltration as analyzed online with a multiangle laser light scattering detector. In contrast, sDPP-IV deglycosylated with EndoF glycosidase shows an uniform molecular weight over the whole peak range, because of the specific cleavage of asparagine linked oligomannose after the first N-acetylglucoamines residue (GlcNAc). This leads to a decrease in molecular weight of 20 kDa as estimated by SDS-PAGE. Crystals

suitable for X-ray diffraction are only observed for deglycosylated sDPP-IV and structure analysis shows four GlcNAc with interpretable electron density at the positions N85, N150, N229 and N281 in subunit A. In subunit B, again N85, N150 and N229 are visible, but no electron density was found for N281 and an additional site could be identified at N92. The GlcNAc of N85 is involved in a crystal contact in both subunits.

DPP-IV expressed in human has a more complex type of glycosylation compared to P. pastoris (Cremata, J., Montensino, R., Quintero, O. & Garcia, R. (1998). Glycosylation Profiling of Heterologous Proteins. In *Pichia Protocols* (Higgins, D.R. & Cregg, J.M., eds.), vol. 103. pp. 95-106, Humana Press: Totowa, New Jersey) and contains terminal sialic acid, however, this seems not to be a requirement for correct folding as shown here.

Interaction with ADA

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Adenosine deaminase (ADA; EC 3.5.4.4) is a 41 kDa protein expressed in all mammaliantissues that catalyzes the deamidation of adenosine and 2'-deoxyadenosine to inosine and 2'-deoxyinosine, respectively. It is important for the regulation of the extracellular concentration of adenosine and for the regulation of the immune response. ADA is involved in T cell activation in general and the pathogensis of autoimmune disorders (such as rheumatoid arthritis) as well as the mechanism of immunodeficiency disease (such as SCID or AIDS). Binding of the soluble extracellular ADA is a unique property of DPP-IV molecules of higher mammals and is not observed in mouse nor rat DPP-IV (Iwaki-Egawa, S., Watanabe, Y. & Fujimoto, Y. (1997). CD26/dipeptidyl peptidase IV does not work as an adenosine deaminase-binding protein in rat cells. *Cell Immunol.* 178, 180-186). Using analytical ultra-centrifugation, we observe a 1:1 complex of a ADA molecules with a sDPP-IV subunit giving a molecular weight of 252 kDa. Surface plasmon resonance (Biacore) measurements show a binding constant of 3.15 ± 2 nM to ADA from bovine with a very low dissociation rate (k_{off} =8.75*10⁻⁵ s⁻¹, k_{on} =2.98*10⁴ M⁻¹s⁻¹) indicating a strong interaction.

Mutagenesis studies (Abbott, C.A., McCaughan, G.W., Levy, M.T., Church, W.B. & Gorrell, M.D. (1999). Binding to human dipeptidyl peptidase IV by adenosine deaminase and antibodies that inhibit ligand binding involves overlapping, discontinuous sites on a predicted beta propeller domain. *Eur. J. Biochem.* 266, 798-810; Dong, R.P., Tachibana, K., Hegen, M., Munakata, Y., Cho, D., Schlossman, S.F. & Morimoto, C. (1997). Determination of adenosine deaminase binding domain on CD26 and its immunoregulatory effect on T cell activation. *J. Immunol.* 159, 6070-6076) identified two important regions in DPP-IV Leu₃₄₀-Val₃₄₁-Ala₃₄₂-Arg₃₄₃ (at the beginning of β5/4) and

Leu294 (α4, at the end of blade 4) and a less important region Glu₃₃₂-Ser₃₃₃-Ser₃₃₄-Gly₃₃₅-Arg₃₃₆ (loop region, at the end of β 5/3) that are all located at the surface of the β -propeller domain (Figure 1). Mutation to amino acids found in rat DPP-IV reduces binding affinity to ADA. These residues form a binding site that is located far away from the active site (Figure 2) confirming the independence of DPP-IV activity on ADA binding (Table 1; De Meester, I., Vanham, G., Kestens, L., Vanhoof, G., Bosmans, E., Gigase, P. & Scharpe, S. (1994). Binding of adenosine deaminase to the lymphocyte surface via CD26. Eur. J. Immunol. 24, 566-570). It is concluded that the function of DPP-IV is the localization and orientation of ADA for proper catalysis. The structure gives an indication for the orientation and localization at the cell surface, because the N-terminus must be close to the membrane and the ADA binding would be on the opposite site of the molecule pointing away from the cell surface (Figure 2). Further, there would be sufficient space enabling interaction of ADA to the A1-adenosine receptor (Ciruela, F., Saura, C., Canela, E.I., Mallol, J., Lluis, C. & Franco, R. (1996). Adenosine deaminase affects ligand-induced signaling by interacting with cell surface adenosine receptors. FEBS Lett. 380, 219-223) which probably plays an important role in the ontogenesis of immune tissues. This view would also support the hypothesis proposing a link for cell-cell interaction via the binding of DPP-IV, ADA and A1-adenosine.

Biological Implications

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The crystal structure of DPP-IV at 2.1 Å resolution reveals a V-shaped dimeric molecule with an extended dimer interface fostering the conformation of the overall molecule. The membrane association and stability of DPP-IV is used for binding of other proteins like ADA in order to achieve localization without disturbance of the enzymatic functionality.

Analysis of the complex with Diprotin A shows key structural features for proline specific exopeptidase specificity and activity. The negative charge of the double Glu motif guides the N-terminus of the peptide to the active site and fixes the substrate in the correct position for cleavage. The distance between this motif and the catalytic Ser630 limits the cleavage to dipeptides and the S1 pocket can just adopt proline or with less affinity alanine as side chains.

The low turnover rate of Diprotin A may be explained by the hydrophobic interaction of the two Ile-residues in the P2 and P1' positions as well as an extensive salt bridge cluster that involves the negatively charged C-terminus of Diprotin A. This structural information will aid the design of new specific inhibitors.

The active site is very accessible to the solvent by two entrances explaining that peptides can be cleaved by DPP-IV with almost no size limitation. A second access to the active site by the tunnel of the β -propeller domain is large enough to enable the release of the cleaved dipeptides. This structural arrangement certainly improves the catalytic turnover and is in great contrast to the crystal structure of POP that shows a much more narrow tunnel and no further access to the active site.

For most of the special features of DPP-IV namely dimerization, regulation of substrate access via two entrances, recognition of the substrate (double Glu-motif) and interaction with other proteins like ADA the β -propeller domain plays a key role. Thus, DPP-IV is an excellent example that the β -propeller fold can be tailored to adapt to different functionality.

Table 1. Enzyme Kinetic Constants of DPP-IV										
proteins	k _{cat} *	K _M *	k_{cat}/K_{M}							
	(s ⁻¹)	μΜ)	μ M ⁻¹ s ⁻¹)							
sDPP-IV _{deglycos}	43.1	17.2	2.51							
$sDPP-IV_{glycos}$	37.3	15.5	2.41							
sDPP-IV _{deglycos.} /ADA	39.6	14.8	2.68							

^{*} analyzed using Lineweaver-Burk plots; buffer: 50 mM Tris/HCl pH 7.8, containing 100 mM NaCl, 0.1 mg/ml BSA and 0.5% Dimethyl-formamid; temperature: 25°C

	K _I	K _D	k _{on}	k _{off}
	μΜ)	μΜ)	$M^{-1}s^{-1}$	s ⁻¹
Ile-Pro-Ile	4.63 [‡]	3.8 [†]	-	-
NVP-DPP728	0.006 ‡	0.002 [†]	1.36*10 ^{6†}	2.48*10 ⁻³ †
NVP-DPP728 _(Lit.)	0.011	0.010	1.3*10 ⁵	1.3*10 ⁻³

[†] measured with biacore; buffer: 0.01 M Hepes, pH 7.4, containing 0.15 M NaCl, 3 mM EDTA, 0.005% polysorbate 20 (v/v)

[‡] temperature: 25°C; in assay buffer (see Table 1); glycosylated sDPP-IV

^{*} Hughes, T.E., Mone, M.D., Russell, M.E., Weldon, S.C. & Villhauer, E.B. (1999). NVP-DPP728 (1-[[[2-[(5-cyanopyridin-2-yl)amino]ethyl]amino]acetyl]-2-cyano-(S)- pyrrolidine), a slow-binding inhibitor of dipeptidyl peptidase IV. *Biochemistry* 38, 11597-11603

Data set	MAD	MAD	MAD	Apo	Diprotin-A
	Remote	Peak	Inflection		complex
Wavelength	0.992	1.0065	1.009	0.9765	0.92
X-ray source	SLS	SLS	SLS	ID14, ESRF	SLS
Detector	MAR IP ^a	MAR IP ^a	MAR IP ^a	Quantum CCD	MAR CCE
Exposure time/frame (s)	10	10	10	2	4
angular increment per frame (°)	2.0	2.0	2.0	0.25	0.25
total rotation range (*)	110	136	140	130	130
crystal to detector distance (mm)	410	410	410	240	260
unit cell parameters a,b,c (Å)	65.2; 68.7;	65.2; 68.7; 420	.165.2; 68.7; 420.1		65.1; 67.1;
	420.1		, ,	419.3	419.6
data reduction					
Maximum Resolution (Å)	2.6	2.6	2.6	2.1	2.5
No. of measurements	212 619	263 910	276 921	. 234 528	171 090
No. of unique reflections	58 627	59 544	59 939	87 113	64 208
completeness (%)*	97.5 (99.4)	99.9 (100.0)	99.9 (99.9)	82.9 (72.3)	97.5 (99.4)
Rsym *, ^{b*}	9.1 (15.9)	9.0 (18.1)	8.6 (14.2)	8.4 (26.8)	9.1(15.9)
heavy-atom refinement paramet					
?(e) / f' (e)	-7.0 / 9.5	-8.0 / 9.8	-12.1 / 5.0		
Phasing power ^c (anomalous)	0.95	1.0	0.7		
Refinement statistics					
resolution range (Å)				20 – 2.1	30 – 2.5
$R_{cryst} (R_{free})^d (\%)$				21.5 (26.5)	22.5 (28.2)
No. of protein atoms ^e (mean B				11 962	11 962 (27.1
n Ų)				(34.6)	•
No. of water molecules				322 (33.4)	268 (25.0)
No. of ligand/heavy atoms				6 (77.3)	24 (28.3)
mean B in Å ²)					r
No. of NAG atoms (mean B in				112 (59.0)	98 (51.4)
h ²)					
msd ^f bonds (Ų)				0.018	0.019
kmsd ^f angles (*)				1.86	2.07

^a Marresearch image plate detector, diameter 345mm, 100µm pixel size

^{&#}x27;Values in parentheses are statistics for highest resolution bin.

 $^{^{}b}$ $R_{sym} = \Sigma_{h} \Sigma_{i} |I_{i}(h) - \langle I(h) \rangle |/\Sigma_{h} \Sigma_{i}(h)$, where $I_{i}(h)$ und $\langle I(h) \rangle$ are the ith and mean measurement of the intensity of reflection h.

^c Phasing power = $\Sigma_h F_H(h)/\Sigma_h |F_D(h) - |F_N(h) + F_H(h)||$.

 $^{^{}d}\Sigma_{h}||F_{obs}|-|F_{calc}||/\Sigma_{h}|F_{obs}|$, where $|F_{obs}|$ and $|F_{calc}|$ are the observed and calculated structure factor amplitudes for the reflection h, applied to the working (R_{cryst}) and test (R_{free})sets, respectively.

^c Non-hydrogen atoms, only.

frmsd: root mean square deviation from mean.

Table 4: Structure coordinates for human DPP-IV

Table 4 lists the atomic structure coordinates for DPP-IV as derived by X-ray diffraction from a crystal of DPP-IV.

```
HEADER
               DPP-IV
               Human Dipeptidyl peptidase IV
    COMPND
     COMPNID
     SOURCE
     REMARK
     REMARK
                 REFINEMENT REMARKS:
    REMARK
     REMARK
              1
    REMARK
              1
                   "apo"-structure
    REMARK
              1
                   (mercury derivative different from MAD experiment used for
     refinement)
    REMARK
              1
    REMARK
    REMARK
    REMARK
                                        2.1A resolution
    REMARK
    REMARK
              3
              3 REFINEMENT.
    REMARK
                  PROGRAM
                               : REFMAC 5.0
    REMARK
              3
                  AUTHORS : MURSHUDOV, VAGIN, DODSON
    REMARK
    REMARK
                   REFINEMENT TARGET : MAXIMUM LIKELIHOOD
    REMARK
    REMARK
                DATA USED IN REFINEMENT.
    REMARK
    REMARK
                 RESOLUTION RANGE HIGH (ANGSTROMS)
                  RESOLUTION RANGE LOW (ANGSTROMS) :
                                                         12.00
    REMARK
    REMARK
              3
                  DATA CUTOFF
                                          (SIGMA(F)) : NONE
                  COMPLETENESS FOR RANGE
                                                         82.99
    REMARK
                                                  (કે) :
    REMARK
                  NUMBER OF REFLECTIONS
                                                          87113
    REMARK
    REMARK
                 FIT TO DATA USED IN REFINEMENT.
              3
                  CROSS-VALIDATION METHOD
                                                     : THROUGHOUT
    REMARK
                  FREE R VALUE TEST SET SELECTION
                                                    : RANDOM
    REMARK
                             (WORKING + TEST SET) : 0.21747
    REMARK
              3
                  R VALUE
    REMARK
              3
                  R VALUE
                                      (WORKING SET)
                                                        0.21485
    REMARK
                  FREE R VALUE
                                                        0.26560
                  FREE R VALUE TEST SET SIZE
    REMARK
              3
                  FREE R VALUE TEST SET COUNT
                                                        4619
    REMARK
              3
    REMARK
    REMARK
                 FIT IN THE HIGHEST RESOLUTION BIN.
    REMARK
                  TOTAL NUMBER OF BINS USED
                                                               20
                                                             2.100
    REMARK
                  BIN RESOLUTION RANGE HIGH
    REMARK
              3
                  BIN RESOLUTION RANGE LOW
                                                             2.153
              3
                  REFLECTION IN BIN
                                         (WORKING SET)
    REMARK
                                                              2014
                                         (WORKING SET)
    REMARK
              3
                  BIN R VALUE
                                                             0.246
    REMARK
              3
                  BIN FREE R VALUE SET COUNT
50
    REMARK
                  BIN FREE R VALUE
    REMARK
                 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
    REMARK
              3
                  ALL ATOMS
    REMARK
              3
                                                  12366
    REMARK
              3
55
                 ESTIMATED OVERALL COORDINATE ERROR.
    REMARK
                  ESU BASED ON R VALUE
                                                                     (A):
                                                                            0.280
    REMARK
                  ESU BASED ON FREE R VALUE
    REMARK
                                                                     (A):
                                                                            0.228
                  ESU BASED ON MAXIMUM LIKELIHOOD
    REMARK
                                                                            0.244
                                                                            9.427
    REMARK
                  ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2):
60
    REMARK
    REMARK
                 RMS DEVIATIONS FROM IDEAL VALUES
                                                           COUNT
                                                                    RMS
                                                                            WEIGHT
    REMARK
                                                      (A): 12400 ; 0.018 ; 0.021
    REMARK
                  BOND LENGTHS REFINED ATOMS
                  BOND LENGTHS OTHERS
                                                      (A): 10588; 0.001; 0.020
    REMARK
                                                (DEGREES): 16876; 1.867; 1.936
                  BOND ANGLES REFINED ATOMS
    REMARK
                                                (DEGREES): 24632; 0.889; 3.000
(DEGREES): 1454; 5.183; 3.000
                  BOND ANGLES OTHERS
    REMARK
    REMARK
                  TORSION ANGLES, PERIOD 1
                  TORSION ANGLES, PERIOD 3
CHIRAL-CENTER RESTRAINTS
                                              (DEGREES):
                                                           2075 ;19.350 ;15.000
    REMARK
                                                   (A**3):
    REMARK
                                                            1790 ; 0.135 ; 0.200
70
    REMARK
                  GENERAL PLANES REFINED ATOMS
                                                      (A): 13738; 0.007; 0.020
                                                      (A): 2674; 0.004; 0.020
(A): 2592; 0.240; 0.300
    REMARK
                  GENERAL PLANES OTHERS
                  NON-BONDED CONTACTS REFINED ATOMS (A):
    REMARK
    REMARK
                  NON-BONDED CONTACTS OTHERS
                                                      (A): 10721; 0.223; 0.300
```

```
REMARK
                     NON-BONDED TORSION OTHERS
                                                         (A):
                                                                 17; 0.494; 0.500
       REMARK
                 3
                     H-BOND (X...Y) REFINED ATOMS
                                                                   ; 0.155 ; 0.500
                                                         (A):
                                                                820
       REMARK
                     H-BOND (X...Y) OTHERS
                                                         (A):
                                                                      0.115
                    SYMMETRY VDW REFINED ATOMS
SYMMETRY VDW OTHERS
SYMMETRY H-BOND REFINED ATOMS
                                                                            : 0.500
       REMARK
                 3
                                                         (A):
                                                                  9
                                                                   ; 0.235 ; 0.300
       REMARK
                 3
                                                         (A):
                                                                38 ; 0.277 ; 0.300
       REMARK
                                                                  3 ;
                                                                     0.397 ; 0.500
                                                         (A):
       REMARK
                3
                    ISOTROPIC THERMAL FACTOR RESTRAINTS.
       REMARK
                3
                                                              COUNT
                                                                       RMS
                                                                              WEIGHT
       REMARK
                3
                    MAIN-CHAIN BOND REFINED ATOMS
                                                     (A**2):
                                                              7252 ; 0.874 ; 1.500
                    MAIN-CHAIN ANGLE REFINED ATOMS (A**2): 11766 ; 1.603
  10
       REMARK
                3
                                                                            ; 2.000
                    SIDE-CHAIN BOND REFINED ATOMS (A**2):
       REMARK
                                                              5148 ; 2.300
                                                                            ; 3.000
                    SIDE-CHAIN ANGLE REFINED ATOMS (A**2):
       REMARK
                3
                                                              5110 ; 3.638 ; 4.500
       REMARK
                3
       REMARK
                3
                   NCS RESTRAINTS STATISTICS
  15
                    NUMBER OF NCS GROUPS : NULL
      REMARK
       REMARK
      REMARK
      REMARK
      REMARK
                    data collected at 100K at ID14 in Grenoble (ESRF, France)
                4
  20
      REMARK
                    Phasing by MAD using Hg derivative and data collected to 2.7 A
                4
      REMARK
                    at Villigen (SLS, Switzerland)
                4
      REMARK
      SEQRES
                1 A
                          SER ARG LYS THR TYR THR LEU THR ASP TYR LEU LYS ASN
                     728
      SEQRES
                2 A
                          THR TYR ARG LEU LYS LEU TYR SER LEU ARG
                     728
                                                                    TRP
                                                                        ILE SER
 25
      SEORES
                3 A
                     728
                          ASP HIS GLU
                                      TYR LEU TYR LYS GLN GLU ASN ASN
                                                                        ILE LEU
      SECRES
                4 A
                     728
                          VAL PHE ASN ALA GLU TYR GLY ASN SER SER VAL PHE LEU
                          GLU ASN SER THR PHE ASP GLU PHE GLY HIS SER ILE ASN
      SEORES
               5 A
                     728
      SEQRES
               6 A
                     728
                          ASP TYR SER
                                      ILE SER PRO ASP GLY GLN PHE ILE LEU LEU
      SEQRES
               7 A
                     728
                          GLU TYR ASN TYR VAL LYS GLN TRP ARG HIS SER TYR
                                                                            THR
 30
      SEQRES
               8 A
                     728
                          ALA SER
                                  TYR ASP
                                          ILE TYR ASP LEU ASN LYS ARG GLN LEU
      SEORES
               9 A
                          ILE THR GLU GLU ARG ILE PRO ASN ASN
                     728
                                                               THR GLN TRP
                                                                            VAL
      SEORES
              10 A
                     728
                          THR TRP
                                  SER PRO VAL GLY HIS LYS LEU ALA TYR VAL
                                                                            TRP
      SEQRES
              11 A
                     728
                          ASN ASN ASP
                                      ILE TYR
                                              VAL LYS ILE
                                                           GLU PRO ASN LEU PRO
      SEQRES
              12
                     728
                          SER TYR ARG ILE THR TRP THR GLY LYS
                                                               GLU ASP
                                                                       ILE
                                                                            ILE
 35
      SEQRES
              13 A
                     728
                          TYR ASN GLY ILE THR ASP TRP VAL
                                                           TYR GLU GLU GLU VAL
      SEQRES
              14 A
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                                                     37.897
                                                               25.546
                                                                        1.00 57.24
      ATOM
                14
                     NE
                          ARG A
                                  40
                                            86.328
                                                     36.534
                                                               25.499
                                                                        1.00 58.28
 30
      ATOM
                                            85.660
                15
                     CZ
                          ARG A
                                  40
                                                     35.448
                                                               25.096
                                                                        1.00 59.61
      ATÓM
                16
                     NH1
                         ARG A
                                  40
                                            84.401
                                                     35.530
                                                               24.686
                                                                        1.00 61.49
      ATOM
                17
                     NH2
                         ARG A
                                  40
                                            86.261
                                                     34.262
                                                               25.094
                                                                        1.00 58.92
      ATOM
                18
                     N
                          LYS A
                                  41
                                            83.456
                                                     41.803
                                                               25.081
                                                                        1.00 48.23
     ATOM
                19
                     CA
                          LYS A
                                  41
                                            82.818
                                                     42.756
                                                                        1.00 46.53
                                                               25.984
 35
     ATOM
                20
                     С
                          LYS A
                                  41
                                            81.370
                                                     42.368
                                                              26.314
                                                                        1.00 44.42
     MOTA
                21
                     0
                          LYS A
                                  41
                                            80.703
                                                     41.655
                                                              25.573
                                                                        1.00 43.94
                                           82.863
82.277
                                                     44.105
45.301
     ATOM
                22
                     CB
                          LYS A
                                  41
                                                              25.282
                                                                        1.00 46.80
     ATOM
                23
                     CG
                          LYS A
                                  41
                                                              25.964
                                                                        1.00 48.40
     ATOM
                                           81.868
                24
                     CD
                          LYS A
                                                     46.280
                                  41
                                                              24.842
                                                                        1.00 48.84
 40
     MOTA
                25
                     CE
                          LYS A
                                                     47.736
48.511
                                  41
                                           82.184
                                                              25.157
                                                                        1.00 51.33
     MOTA
                26
                     NZ
                          LYS A
                                  41
                                           82.581
                                                              23.903
                                                                        1.00 53.12
     ATOM
                                           80.885
                27
                     N
                          THR A
                                  42
                                                     42.833
                                                              27.447
                                                                        1.00 41.70
     MOTA
                28
                     CA
                          THR A
                                  42
                                           79.609
                                                     42.354
                                                              27.944
                                                                        1.00 39.43
     MOTA
                29
                     C
                          THR A
                                           78.630
                                  42
                                                     43.494
                                                              28.003
                                                                        1.00 37.10
45
     ATOM
                30
                     0
                          THR A
                                  42
                                           79.076
                                                              27.942
                                                     44.650
                                                                        1.00 36.72
     ATOM
                31
                                           79.896
                     CB
                         THR A
                                  42
                                                                        1.00 39.73
                                                     41.729
                                                              29.310
     MOTA
                32
                     OG1
                         THR A
                                  42
                                           79.355
                                                     40.410
                                                              29.352
                                                                        1.00 40.73
     ATOM
                33
                     CG2
                         THR A
                                  42
                                           79.301
                                                     42.522
                                                              30.430
                                                                        1.00 37.70
                                           77.317
76.299
     ATOM
                34
                     N
                          TYR A
                                  43
                                                     43.203
44.283
                                                              28.044
                                                                        1.00 34.78
50
     MOTA
                35
                     CA
                         TYR A
                                  43
                                                              28.125
                                                                        1.00 33.64
     ATOM
                36
                     С
                         TYR A
                                  43
                                           76.198
                                                     44.822
                                                              29.571
                                                                        1.00
                                                                             32.40
     ATOM
                37
                     0
                         TYR A
                                  43
                                           75.706
                                                     44.146
                                                              30.453
                                                                        1.00 29.56
     ATOM
                38
                     CB
                         TYR A
                                  43
                                           74.918
                                                     43.829
                                                              27.617
                                                                        1.00
                                                                             33.75
     ATOM
                39
                                                    44.942
45.770
                                                              27.562
26.453
                     CG
                         TYR A
                                  43
                                           73.894
                                                                       1.00
                                                                             32.19
55
     ATOM
                40
                     CD1
                         TYR A
                                 43
                                           73.804
                                                                       1.00
                                                                             31.74
     ATOM
                41
                     CD2 TYR A
                                 43
                                           72.986
                                                     45.146
                                                              28.603
                                                                       1.00
                                                                             31.84
     MOTA
                42
                     CE1
                         TYR A
                                 43
                                           72.874
                                                    46.782
                                                              26.373
                                                                       1.00 30.93
     ATOM
                43
                     CE2
                         TYR A
                                           72.047
                                                              28.533
27.408
                                 43
                                                     46.157
                                                                       1.00 29.54
     ATOM
                44
                     cz
                                           71.978
                         TYR A
                                 43
                                                    46.965
                                                                       1.00
                                                                             31.35
60
     ATOM
                45
                    OH
                         TYR A
                                 43
                                           71.044
                                                    48.003
                                                              27.358
                                                                       1.00
                                                                             31.31
     ATOM
                46
                    N
                         THR A
                                 44
                                           76.629
                                                    46.056
                                                              29.758
                                                                       1.00
                                                                             32.15
     MOTA
                47
                    CA
                         THR A
                                 44
                                           76.897
                                                    46.588
                                                              31.100
                                                                       1.00 33.67
     ATOM
               48
                    C
                         THR A
                                 44
                                           75.766
                                                    47.433
                                                              31.694
                                                                       1.00
                                                                             32.40
     MOTA
               49
                    0
                         THR A
                                           74.842
                                 44
                                                    47.835
                                                              30.988
                                                                       1.00
                                                                             31.22
65
               50
     MOTA
                    СВ
                         THR A
                                 44
                                           78.193
                                                    47.433
                                                              31.066
                                                                       1.00 33.26
     MOTA
               51
                    OG1
                         THR A
                                 44
                                           79.329
                                                    46.619
                                                              30.661
                                                                       1.00 39.41
     MOTA
               52
                    CG2
                         THR A
                                 44
                                           78.592
                                                    47.767
                                                              32.396
                                                                       1.00
                                                                             36.50
     MOTA
               53
                         LEU A
                                                    47.711
                    N
                                 45
                                           75.859
                                                              32.989
                                                                       1.00
                                                                             31.13
     MOTA
               54
                    CA
                         LEU A
                                 45
                                           74.864
                                                    48.531
                                                              33.618
                                                                             30.66
                                                                       1.00
70
    MOTA
               55
                    С
                                 45
                                                    49.885
                         LEU A
                                           74.926
                                                              32.988
                                                                       1.00
                                                                            30.59
    ATOM
               56
                    0
                         LEU A
                                 45
                                           73.880
                                                    50.426
                                                             32.631
                                                                       1.00 30.36
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	ATOM ATOM ATOM	57 58 59	CB CG CD1	LEU A LEU A LEU A	45 45 45	75.080 74.141 72.682	48.633 49.585 49.261	35.113 35.847 35.589	1.00	31.36 30.22 32.27
5	ATOM ATOM ATOM	60 61 62	CD2 N CA	THR A	45 46 46	74.430 76.132 76.279	49.492 50.425 51.719	37.345 32.818 32.170	1.00	29.39 29.60 30.54 30.14
10	ATOM ATOM ATOM ATOM	63 64 65 66	C O CB OG1	THR A THR A THR A THR A	46 46 46 46	75.693 75.083 77.758 78.263	51.704 52.682 52.173 52.477	30.747 30.318 32.102 33.401	1.00 1.00	30.14 30.45 30.74 30.83
	ATOM ATOM ATOM	67 68 69	CG2 N CA	THR A ASP A ASP A	46 47 47	77.855 75.874 75.344	53.537 50.598 50.455	31.420 30.031 28.666	1.00 1.00 1.00	32.16 30.76 31.14
15	ATOM ATOM ATOM ATOM	70 71 72 73	C O CB CG	ASP A ASP A ASP A	47 47 47 47	73.841 73.303 75.630 77.082	50.702 51.474 49.064 48.892	28.685 27.910 28.116 27.660	1.00 1.00	31.39 32.18 30.01 29.29
20	ATOM ATOM ATOM	74 75 76	OD1 OD2 N	ASP A ASP A TYR A	47 47 48	77.714 77.672 73.179	49.894 47.793 50.083	27.275 27.663 29.643	1.00 1.00 1.00	28.27 24.95 31.92
	ATOM ATOM ATOM ATOM	77 78 79 80	CA C O CB	TYR A TYR A TYR A TYR A	48 48 48 48	71.745 71.353 70.493 71.264	50.232 51.637 52.230 49.307	29.770 30.150 29.567 30.847		31.38 31.54 29.15 31.04
25	ATOM ATOM ATOM	81 82 83	CG CD1 CD2	TYR A TYR A TYR A	48 48 48	69.857 68.846 69.554	49.596 49.629 49.874	31.233 30.284 32.529	1.00 1.00 1.00	28.68 27.94 29.63
30	ATOM ATOM ATOM ATOM	84 85 86 87	CE1 CE2 CZ OH	TYR A TYR A TYR A TYR A	48 48 48 48	67.534 68.242 67.229 65.943	49.907 50.126 50.153 50.438	30.636 32.930 31.984 32.420	1.00 1.00 1.00	32.09 31.86 32.29 31.53
35	ATOM ATOM ATOM	88 89 90 91	N CA C	LEU A LEU A	49 49 49 49	72.020 71.725 72.100 71.456	52.160 53.485 54.588 55.643	31.155 31.669 30.697 30.660	1.00 1.00	32.84 34.60 35.66 34.88
55	ATOM ATOM ATOM ATOM	92 93 94	O CB CG CD1	LEU A LEU A LEU A	49 49 49	72.533 71.926 70.447	53.695 53.503 52.989	32.944 34.334 34.355	1.00 1.00	34.83 37.04 37.50
40	ATOM ATOM ATOM ATOM	95 96 97 98	CD2 N CA C	LEU A LYS A LYS A	49 50 50 50	72.853 73.161 73.625 73.139	52.643 54.374 55.444 55.299	35.176 29.922 29.055 27.618	1.00	37.79 36.93 39.10 40.54
45	ATOM ATOM ATOM	99 100 101	O CB CG	LYS A LYS A LYS A	50 50 50	73.333 75.147 75.559	56.202 55.568 55.978	26.789 29.166 30.583	1.00	39.65 39.68 41.11
	ATOM ATOM ATOM	102 103 104	CD CE NZ	LYS A LYS A	50 50 50	74.992 75.551 75.091	57.392 57.976 59.395	30.909 32.226 32.481	1.00	43.27 45.34 44.42
50	ATOM ATOM ATOM ATOM	105 106 107 108	N CA C O	ASN A ASN A ASN A	51 51 51 51	72.470 71.929 73.048 73.003	54.165 53.851 53.801 54.506	27.363 26.061 25.038 24.069	1.00 1.00	41.96 43.12 43.29 43.46
55	ATOM ATOM ATOM ATOM	109 110 111 112		ASN A ASN A ASN A	51 51 51 51	70.928 69.665 69.127 69.151	54.919 54.976 53.945 56.193	25.603 26.443 26.903 26.616	1.00 1.00	43.38 46.23 48.91 44.86
	ATOM ATOM ATOM	113 114 115	N CA C	THR A THR A THR A	52 52 52	74.038 75.150 74.698	52.954 52.802 52.189	25.254 24.336 23.020	1.00 1.00 1.00	44.16 44.31 44.61
60	ATOM ATOM ATOM ATOM	116 117 118 119	O CB OG1 CG2		52 52 52 52	75.284 76.166 76.595 77.446	52.429 51.790 52.157 51.804	21.971 24.900 26.200 24.084	1.00 1.00	43.95 44.63 44.54 44.92
65	ATOM ATOM ATOM ATOM	120 121 122 123	N CA C O	TYR A TYR A TYR A TYR A	53 53 53 53	73.707 73.225 71.765 70.856	51.314 50.540 50.895 50.359	23.125 22.003 21.754 22.395	1.00 1.00 1.00 1.00	44.37 43.98 43.98 44.20
70	ATOM ATOM ATOM	124 125 126	CB CG CD1	TYR A TYR A TYR A	53 53 53	73.388 74.835 75.744	49.068 48.621 48.545	22.344 22.567 21.521	1.00	43.63 43.01 39.95

	ATOM ATOM ATOM ATOM	128 (129 (CD2 TYR A CE1 TYR A CE2 TYR A CZ TYR A	53 53	75.277 77.071 76.574	48.119 47.801	23.840 21.740 24.062	1.00 38.67 1.00 41.06
5		131 (132 1 133 (OH TYR A N ARG A CA ARG A C ARG A	53 54 54	77.471 78.754 71.538 70.188 69.433	47.311 51.831 52.335	23.009 23.258 20.841 20.571	1.00 41.11 1.00 37.02 1.00 44.11 1.00 44.03
10	MOTA	135 (136 (137 (D ARG A CB ARG A CG ARG A CD ARG A	54 54 54	70.021 70.279 70.626 70.507	51.014 53.764 54.779	19.553 18.600 20.036 21.120	1.00 42.21 1.00 41.54 1.00 45.08 1.00 51.23
15	ATOM ATOM ATOM ATOM	139 N 140 C 141 N	NE ARG A CZ ARG A NH1 ARG A NH2 ARG A	54 54 54	70.307 71.033 70.352 69.074 70.958	57.116 57.501 57.152	20.718 21.796 22.887 23.064 23.806	1.00 56.63 1.00 61.87 1.00 65.60 1.00 66.87 1.00 66.50
20	ATOM ATOM ATOM ATOM	143 N	N LEU A CA LEU A C LEU A	55 55	68.145 67.256 66.805 66.299	51.285	19.790 18.818 17.946 18.459	1.00 40.64 1.00 40.22 1.00 39.01 1.00 39.01
	ATOM ATOM ATOM ATOM	148 C 149 C 150 C	CB LEU A CG LEU A CD1 LEU A CD2 LEU A	55 55 55	65.976 65.960 64.533 66.447	50.151 48.891 48.667 47.705	19.461 20.292 20.703 19.493	1.00 40.01 1.00 40.34 1.00 42.07 1.00 40.99
. 25	ATOM ATOM ATOM	153 C 154 O	A LYS A LYS A LYS A	56 56 56	66.977 66.403 64.947 64.572	51.709 52.735 52.390 51.223	16.641 15.760 15.492 15.475	1.00 38.06 1.00 37.23 1.00 35.67 1.00 33.89
30	ATOM ATOM ATOM ATOM	156 C 157 C 158 C	D LYS A E LYS A	56 56 56	67.153 68.642 69.188 70.602	52.841 53.149 54.004 53.570	14.441 14.570 13.350 12.876	1.00 37.02 1.00 40.24 1.00 45.04 1.00 46.95
35	ATOM ATOM ATOM	159 N 160 N 161 C 162 C	LEU A A LEU A LEU A	56 57 57 57	70.582 64.165 62.723 62.393	52.395 53.431 53.375 54.023	11.891 15.248 15.048 13.711	1.00 48.99 1.00 35.61 1.00 35.84 1.00 34.84
40	ATOM ATOM ATOM ATOM ATOM ATOM ATOM		B LEU A G LEU A D1 LEU A D2 LEU A	57 57 57 57 57 58	61.272 61.679	54.595 54.211 53.711 54.531 52.265	13.092 16.149 17.602 18.559 17.647	1.00 34.28 1.00 36.81 1.00 40.98 1.00 43.05 1.00 45.26
45	ATOM ATOM ATOM ATOM	169 C 170 C 171 O 172 C	A TYR A TYR A TYR A B TYR A	58 58 58 58	61.132 60.651 59.214 58.252 60.725	53.959 54.643 55.080 54.433 53.744	13.294 12.104 12.403 12.024 10.834	1.00 33.45 1.00 32.51 1.00 32.52 1.00 31.59 1.00 31.99
50	ATOM ATOM ATOM ATOM ATOM	175 CI 176 CI	D1 TYR A	58 58 58 58 58	60.721 59.532 61.920 59.498 61.905	54.535 55.003 54.846 55.751 55.594	9.547 9.017 8.867 7.824 7.651	1.00 31.12 1.00 30.51 1.00 32.94 1.00 29.91 1.00 29.33
55	ATOM ATOM ATOM ATOM ATOM	178 C2 179 OF 180 N 181 C2 182 C	Z TYR A H TYR A SER A	58 58 59 59 59	60.683 60.582 59.089 57.804 57.343	56.039 56.782 56.188 56.732 57.664	7.163 6.032 13.114 13.509 12.452	1.00 30.84 1.00 32.25 1.00 32.95 1.00 32.96 1.00 32.63
60	ATOM ATOM ATOM ATOM	183 O 184 CE 185 OG 186 N	SER A SER A SER A LEU A	59 59 59 60	57.984 57.949 58.527 56.232	58.673 57.434 56.484 57.311	12.171 14.846 15.747 11.842	1.00 33.29 1.00 33.95 1.00 36.22 1.00 31.26
65	ATOM ATOM ATOM ATOM ATOM	187 CA 188 C 189 O 190 CE 191 CG	LEU A LEU A LEU A	60 60 60	55.727 54.307 53.623 55.850	58.068 58.510 57.907 57.211	10.744 11.018 11.800 9.458	1.00 31.83 1.00 31.39 1.00 31.01 1.00 31.26
UJ.	ATOM ATOM ATOM ATOM	192 CD	01 LEU A 02 LEU A ARG A	60 60 61	54.798 55.544 53.669 53.875	56.366 55.212 55.791 59.568	8.730 7.978 9.492 10.352	1.00 32.72 1.00 32.95 1.00 30.55 1.00 32.40
70	ATOM	196 C	ARG A ARG A	61 61	52.511 51.777	60.032 60.077	10.491 9.127	1.00 33.55 1.00 32.37

	ATOM ATOM ATOM	197 198 199	O CB CG	ARG A ARG A ARG A	61 61 61	52.057 52.524 53.286	60.942 61.429 61.606	8.303 11.117 12.500	1.00 31.77 1.00 34.89 1.00 39.34
5	ATOM ATOM ATOM	200 201 202	CD NE CZ	ARG A ARG A ARG A	61 61 61	52.946 53.746 53.610	62.994 63.318 64.448	13.190 14.376 15.089	1.00 44.62 1.00 50.16 1.00 52.70
10	ATOM ATOM ATOM ATOM	203 204 205 206	NH1 NH2 N CA	ARG A ARG A TRP A TRP A	61 61 62 62	52.722 54.379 50.840 50.101	65.363 64.680 59.171 59.222	14.729 16.147 8.877 7.613	1.00 53.04 1.00 54.30 1.00 31.29 1.00 31.61
10	ATOM ATOM ATOM	207 208 209	C O CB	TRP A TRP A TRP A	62 62 62	49.282 48.679 49.159	60.518 60.886 58.028	7.540 8.541 7.468	1.00 32.94 1.00 33.73 1.00 30.78
15	ATOM ATOM ATOM	210 211 212	CG CD1 CD2	TRP A TRP A TRP A	62 62 62	49.815 49.909 50.452	56.694 55.690 56.191	7.295 8.221 6.111 7.679	1.00 28.26 1.00 28.81 1.00 26.95 1.00 26.42
20	ATOM ATOM ATOM ATOM	213 214 215 216	NE1 CE2 CE3 CZ2	TRP A TRP A TRP A TRP A	62 62 62 62	50.567 50.911 50.697 51.573	54.600 54.887 56.721 54.123	6.392 4.835 5.468	1.00 26.42 1.00 21.80 1.00 27.04 1.00 23.60
	ATOM ATOM ATOM	217 218 219	CZ3 CH2 N	TRP A TRP A ILE A	62 62 63	51.353 51.804 49.293	55.951 54.665 61.219	3.924 4.251 6.398	1.00 25.98 1.00 23.38 1.00 32.81
25	ATOM ATOM ATOM ATOM	220 221 222 223	CA C O CB	ILE A ILE A ILE A	63 63 63 63	48.442 47.425 46.623 49.201	62.378 62.160 63.047 63.689	6.202 5.121 4.865 5.868	1.00 33.78 1.00 33.73 1.00 34.24 1.00 34.14
30	ATOM ATOM ATOM	224 225 226	CG1 CG2 CD1	ILE A ILE A ILE A	63 63 63	50.038 50.039 51.006	63.552 64.100 64.668	4.604 7.046 4.426	1.00 34.97 1.00 35.73 1.00 35.37
	ATOM ATOM ATOM	227 228 229	N CA C	SER A SER A	64 64	47.466 46.484 46.523	61.022 60.751 59.285	4.452 3.424 3.113	1.00 33.90 1.00 34.57 1.00 34.76 1.00 33.73
35	ATOM ATOM ATOM ATOM	230 231 232 233	O CB OG N	SER A SER A SER A ASP A	64 64 65	47.091 46.730 47.912 45.885	58.506 61.583 61.164 58.905	3.861 2.159 1.494 2.021	1.00 35.73 1.00 35.22 1.00 36.37 1.00 35.24
40	ATOM ATOM ATOM	234 235 236	CA C O	ASP A ASP A ASP A	65 65 65	45.871 47.214 47.463	57.519 57.090 55.895	1.626 1.102 1.025	1.00 36.01 1.00 34.80 1.00 35.68
	ATOM ATOM ATOM ATOM	237 238 239 240		ASP A ASP A ASP A	65 · 65 65	44.807 44.905 45.448 44.438	57.283 58.287 59.403 58.053	0.549 -0.607 -0.383 -1.762	1.00 36.24 1.00 40.58 1.00 44.21 1.00 44.77
45	ATOM ATOM ATOM	241 242 243	N CA C	HIS A HIS A	66 66 66	48.065 49.333 50.612	58.052 57.704 58.510	0.756 0.123 0.502	1.00 44.77 1.00 34.26 1.00 34.12 1.00 33.56
50	ATOM ATOM	244 245 246	CB CG	HIS A HIS A	66 66	51.687 49.130 48.904	57.697 59.053	-0.053 -1.392 -1.966	1.00 34.13 1.00 37.13
	ATOM ATOM ATOM ATOM	247 248 249 250	CD2 CE1	HIS A HIS A HIS A	66 66 66	47.755 49.681 47.842 48.999	59.778 59.826 60.947 61.003	-1.723 -2.760 -2.337 -2.975	1.00 39.30 1.00 39.35 1.00 42.55 1.00 41.85
55	ATOM ATOM ATOM	251 252 253	N CA C	GLU A GLU A GLU A	67 67 67	50.525 51.679 51.826	59.434 60.192 60.118	1.455 1.908 3.419	1.00 31.81 1.00 31.27 1.00 30.54
60	ATOM ATOM ATOM	254 255 256	O CB CG	GLU A GLU A	67 67 67	50.830 51.592 51.635	59.974 61.675 62.014	4.152 1.534 0.057	1.00 27.91 1.00 31.52 1.00 34.42
	ATOM ATOM ATOM ATOM	257 258 259 260		GLU A GLU A GLU A TYR A	67 67 67 68	51.862 51.272 52.662 53.078	63.498 64.312 63.867 60.194	-0.160 0.589 -1.046 3.882	1.00 39.59 1.00 43.25 1.00 43.29 1.00 30.78
65	ATOM ATOM ATOM	261 262 263	CA C O	TYR A TYR A TYR A	68 68 68	53.349 54.434 55.267	60.283 61.302 61.578	5.313 5.593 4.717	1.00 31.62 1.00 32.69 1.00 31.58
70	ATOM ATOM ATOM	264 265 266	CB CG CD1	TYR A TYR A TYR A	68 68 68	53.688 54.984 56.212	58.928 58.248 58.660	5.934 5.506 6.002	1.00 31.56 1.00 30.01 1.00 28.17

ATOM 271 OH TYR A 68 58.550 56.280 4.371 1.00 31 ATOM 272 N LEU A 69 54.400 61.860 6.810 1.00 31 ATOM 273 CA LEU A 69 55.400 61.860 6.810 1.00 31 ATOM 274 C LEU A 69 55.450 62.728 8.184 1.00 36 ATOM 275 C LEU A 69 55.359 62.028 8.184 1.00 36 ATOM 276 C B LEU A 69 55.947 61.095 8.862 1.00 36 ATOM 277 CG LEU A 69 55.947 61.095 8.862 1.00 36 ATOM 277 CG LEU A 69 53.890 64.916 7.246 1.00 35 ATOM 278 CD1 LEU A 69 53.890 64.916 7.246 1.00 35 ATOM 279 CD2 LEU A 69 53.290 66.024 8.122 1.00 37 ATOM 279 CD2 LEU A 69 54.667 63.958 8.060 1.00 35 ATOM 279 CD2 LEU A 69 54.687 65.522 6.120 1.00 37 ATOM 280 N TYR A 70 57.642 62.392 8.132 1.00 39 ATOM 281 CA TYR A 70 58.696 61.726 8.897 1.00 41 ATOM 281 CA TYR A 70 58.696 61.726 8.897 1.00 44 ATOM 283 O TYR A 70 60.156 63.617 8.490 1.00 43 ATOM 285 CG TYR A 70 60.156 63.617 8.490 1.00 44 ATOM 285 CG TYR A 70 60.250 58.923 9.740 1.00 44 ATOM 287 CD2 TYR A 70 60.250 58.923 9.740 1.00 42 ATOM 286 CD1 TYR A 70 60.250 58.923 9.740 1.00 42 ATOM 289 CE2 TYR A 70 61.792 59.957 8.267 1.00 42 ATOM 289 CE2 TYR A 70 62.826 59.218 8.823 1.00 43 ATOM 290 CZ TYR A 70 62.826 59.218 8.823 1.00 43 ATOM 290 CZ TYR A 70 62.564 58.351 9.893 9.740 1.00 42 ATOM 280 CZ TYR A 70 62.564 58.351 9.893 9.740 1.00 42 ATOM 280 CZ TYR A 70 62.564 58.351 9.893 9.740 1.00 42 ATOM 280 CZ TYR A 70 62.564 58.351 9.893 9.740 1.00 42 ATOM 280 CZ TYR A 70 62.564 59.218 8.823 1.00 43 ATOM 290 CZ TYR A 70 62.564 59.218 8.823 1.00 43 ATOM 290 CZ TYR A 70 62.564 59.218 8.823 1.00 43 ATOM 290 CZ TYR A 70 62.564 69.054 1.00 59. 800 1.00 50 ATOM 290 CZ TYR A 70 66.576 62.793 1.00 50.582 1.00 50 ATOM 290 CZ TYR A 70 66.554 60.054 1.00 50 ATOM 290 CZ TYR A 70 66.554 60.054 1.00 50 ATOM 290 CZ TYR A 70 66.554 60.054 1.00 50 ATOM 290 CZ TYR A 70 66.565 60.618 1.00 50 ATOM 290 CZ TYR A 70 66.565 60.618 1.00 50 ATOM 290 CZ TYR A 70 66.565 60.618 1.00 50 ATOM 290 CZ TYR A 70 66.565 60.618 1.00 50 ATOM 290 CZ TYR A 70 66.565 60.618 1.00 50 ATOM 290 CZ TYR A 70 66.565 60.618 60.618 1.00 50 ATOM 290 CZ TYR A 70 66.565 60.618 60.618 1		ATOM ATOM ATOM	267 CD2 TYR A 268 CE1 TYR A 269 CE2 TYR A	68 68	54.964 57.411 56.142	1 58.000 2 56.493	5.635 4.245	1.00 26.63
ATOM 275 C LEU A 69 56.359 62.028 8.184 1.00 36 ATOM 275 C LEU A 69 55.947 61.095 8.862 1.00 36 ATOM 276 CB LEU A 69 55.947 61.095 8.862 1.00 36 ATOM 277 CG LEU A 69 54.767 63.958 8.060 1.00 35 ATOM 278 CD1 LEU A 69 53.889 64.916 7.246 1.00 35 ATOM 279 CD2 LEU A 69 53.889 64.916 7.246 1.00 35 ATOM 279 CD2 LEU A 69 53.899 66.924 8.122 1.00 37 ATOM 280 N TYR A 70 57.642 62.392 8.132 1.00 39 ATOM 281 CA TYR A 70 57.642 62.392 8.132 1.00 39 ATOM 283 O TYR A 70 59.715 62.785 9.305 1.00 44 ATOM 283 O TYR A 70 59.715 62.785 9.305 1.00 44 ATOM 283 O TYR A 70 60.156 63.617 8.899 1.00 43 ATOM 284 CB TYR A 70 59.715 62.785 9.305 1.00 44 ATOM 285 CG TYR A 70 60.490 99.832 8.721 1.00 41 ATOM 285 CG TYR A 70 60.490 99.832 8.721 1.00 41 ATOM 285 CG TYR A 70 60.490 99.832 8.721 1.00 41 ATOM 285 CG TYR A 70 60.490 99.832 8.721 1.00 41 ATOM 285 CG TYR A 70 60.490 99.832 8.721 1.00 41 ATOM 285 CG TYR A 70 60.490 99.832 8.721 1.00 41 ATOM 285 CG TYR A 70 60.490 99.832 8.721 1.00 41 ATOM 285 CG TYR A 70 60.590 58.923 9.740 1.00 42 ATOM 286 CD1 TYR A 70 60.590 58.923 9.740 1.00 42 ATOM 280 CC2 TYR A 70 62.564 58.351 9.847 1.00 43 ATOM 280 CC2 TYR A 70 62.564 58.351 9.847 1.00 43 ATOM 290 CZ TYR A 70 62.866 59.218 8.823 1.00 43 ATOM 290 CZ TYR A 70 62.866 59.218 8.823 1.00 43 ATOM 293 CA LYS A 71 60.057 62.793 10.582 1.00 43 ATOM 295 CA LYS A 71 60.980 63.806 11.069 1.00 43 ATOM 295 CA LYS A 71 60.980 63.806 11.069 1.00 53 ATOM 295 CB LYS A 71 60.980 63.806 11.069 1.00 53 ATOM 295 CB LYS A 71 60.980 63.806 11.069 1.00 53 ATOM 295 CB LYS A 71 60.980 63.806 11.069 1.00 53 ATOM 295 CB LYS A 71 60.980 63.806 11.069 1.00 50 ATOM 295 CB LYS A 71 60.980 63.806 11.069 1.00 50 ATOM 295 CB LYS A 71 60.980 63.806 11.069 1.00 50 ATOM 295 CB LYS A 71 60.980 63.806 11.069 1.00 50 ATOM 295 CB LYS A 71 60.980 63.806 11.069 1.00 50 ATOM 295 CB LYS A 71 60.980 63.806 11.069 1.00 50 ATOM 295 CB LYS A 71 60.980 63.806 11.069 1.00 50 ATOM 295 CB LYS A 71 60.980 63.806 11.069 1.00 50 ATOM 295 CB LYS A 71 60.980 63.806 11.069 1.00 50 ATOM 295 CB LYS A 71 6	5	ATOM	272 N LEU A	69	58.55(54.40(56.280 61.860	4.371 6.810	1.00 30.35 1.00 33.87
ATOM 279 CD2 LEU A 69 54.687 65.522 6.120 1.00 37 10 ATOM 281 CA TYR A 70 57.642 62.392 8.132 1.00 37 ATOM 281 CA TYR A 70 57.642 62.392 8.132 1.00 31 ATOM 282 C TYR A 70 59.715 62.785 8.897 1.00 41 ATOM 283 O TYR A 70 60.156 63.617 8.490 1.00 43 ATOM 283 C TYR A 70 60.156 63.617 8.490 1.00 43 ATOM 285 CG TYR A 70 60.156 63.617 8.490 1.00 43 ATOM 285 CG TYR A 70 60.490 59.832 8.721 1.00 41 ATOM 285 CG TYR A 70 60.490 59.832 8.721 1.00 41 ATOM 285 CG TYR A 70 60.490 59.832 8.721 1.00 41 ATOM 285 CG TYR A 70 60.490 59.832 8.721 1.00 41 ATOM 285 CG TYR A 70 60.250 58.8923 9.740 1.00 42 ATOM 286 CD1 TYR A 70 61.70 59.715 8.267 1.00 42 ATOM 288 CE1 TYR A 70 61.274 58.190 10.309 1.00 43 ATOM 280 CE2 TYR A 70 62.866 59.218 8.823 1.00 43 ATOM 280 CZ TYR A 70 62.866 59.218 8.823 1.00 43 ATOM 280 CZ TYR A 70 63.594 57.643 10.399 1.00 43 ATOM 293 CA LYS A 71 60.957 62.793 10.582 1.00 43 ATOM 293 CA LYS A 71 60.957 62.793 10.582 1.00 43 ATOM 294 C LYS A 71 60.956 63.806 11.069 1.00 52 ATOM 295 C LYS A 71 62.846 63.808 11.069 1.00 52 ATOM 295 C LYS A 71 62.846 63.808 11.069 1.00 54 ATOM 298 CD LYS A 71 62.564 63.608 13.478 1.00 56 ATOM 299 CE LYS A 71 62.564 63.608 13.478 1.00 56 ATOM 299 CE LYS A 71 59.946 63.608 13.478 1.00 56 ATOM 299 CE LYS A 71 59.946 63.608 13.478 1.00 56 ATOM 299 CE LYS A 71 59.417 64.468 14.680 1.00 63 ATOM 299 CE LYS A 71 59.417 64.468 14.680 1.00 56 ATOM 299 CE LYS A 71 59.417 64.468 14.680 1.00 56 ATOM 299 CE LYS A 71 59.417 64.468 14.680 1.00 56 ATOM 300 NZ LYS A 71 59.417 64.468 14.680 1.00 56 ATOM 300 NZ LYS A 71 59.417 64.468 14.680 1.00 56 ATOM 300 NZ LYS A 71 59.417 64.468 14.680 1.00 56 ATOM 300 NZ LYS A 71 59.66 64.259 10.833 10.833 1.00 59 ATOM 300 NZ LYS A 71 59.417 64.468 14.680 1.00 55 ATOM 300 NZ LYS A 71 59.66 64.79 11.00 54 ATOM 300 NZ LYS A 71 59.66 64.79 11.00 54 ATOM 300 NZ LYS A 71 59.66 64.250 64.235 10.833 1.00 59 ATOM 300 NZ LYS A 71 59.66 64.79 11.00 50 ATOM 300 NZ LYS A 71 59.66 64.79 11.00 50 ATOM 300 NZ LYS A 71 59.66 64.79 11.00 50 ATOM 300 NZ LYS A 71 59.66 64.79 11.00	10	MOTA MOTA MOTA	275 O LEU A 276 CB LEU A 277 CG LEU A	69 69 69	56.359 55.947 54.767 53.889	62.028 61.095 63.958 64.916	8.184 8.862 8.060 7.246	1.00 36.95 1.00 36.55 1.00 35.63 1.00 35.92
ATOM 284 CB TYR A 70 60.156 63.617 8.490 1.00 43 ATOM 285 CG TYR A 70 60.490 59.832 8.721 1.00 41 ATOM 286 CD TYR A 70 60.490 59.832 8.721 1.00 41 ATOM 287 CD2 TYR A 70 60.250 58.923 9.740 1.00 42 ATOM 288 CEI TYR A 70 61.274 58.190 10.309 1.00 42 ATOM 289 CEI TYR A 70 61.274 58.190 10.309 1.00 42 ATOM 289 CEI TYR A 70 62.866 59.218 8.823 1.00 43. ATOM 290 CZ TYR A 70 62.866 59.218 8.823 1.00 43. ATOM 291 OH TYR A 70 63.594 57.643 10.399 1.00 43. ATOM 292 N LYS A 71 60.980 63.806 11.069 1.00 52. ATOM 293 CA LYS A 71 60.980 63.806 11.069 1.00 52. ATOM 294 C LYS A 71 60.980 63.806 11.069 1.00 54. ATOM 295 C LYS A 71 62.560 62.450 12.201 1.00 54. ATOM 296 CB LYS A 71 60.496 64.499 12.359 1.00 53. ATOM 297 CG LYS A 71 59.964 63.608 13.478 1.00 56. ATOM 298 CE LYS A 71 59.964 63.608 13.478 1.00 56. ATOM 299 CE LYS A 71 59.964 63.608 13.478 1.00 56. ATOM 300 NZ LYS A 71 59.417 64.468 14.680 1.00 60. ATOM 301 N GLN A 72 66.466 63.082 10.317 1.00 54. ATOM 302 CA GLN A 72 66.366 62.331 10.304 10.306 1.00 66. ATOM 303 C GLN A 72 66.466 63.082 10.317 1.00 58. ATOM 304 O GLN A 72 66.466 63.082 10.317 1.00 58. ATOM 307 CD GLN A 72 66.506 62.331 10.843 1.00 56. ATOM 309 NZ LYS A 71 66.596 64.235 10.843 1.00 56. ATOM 309 NZ LYS A 71 66.596 64.235 10.843 1.00 56. ATOM 301 N GLN A 72 66.506 62.337 8.905 1.00 58. ATOM 303 C GLN A 72 66.506 61.386 10.371 1.00 57. ATOM 305 CB GLN A 72 66.506 61.381 10.306 1.00 58. ATOM 307 CD GLN A 73 66.256 61.396 11.872 1.00 58. ATOM 309 NZ LYS A 71 59.968 63.976 11.872 1.00 59. ATOM 310 N GLU A 73 66.256 61.238 6.511 10.306 1.00 59. ATOM 310 N GLU A 73 66.256 61.238 6.611 10.306 1.00 59. ATOM 310 N GLU A 73 66.256 61.238 6.611 10.00 59. ATOM 310 N GLU A 73 66.256 61.238 6.611 10.00 59. ATOM 310 N GLU A 73 66.256 61.238 6.611 10.00 59. ATOM 310 N GLU A 73 66.256 61.238 6.611 10.00 59. ATOM 310 N GLU A 73 66.256 61.238 6.611 10.00 59. ATOM 310 CB GLU A 73 69.508 63.976 11.872 1.00 59. ATOM 310 N GLU A 73 69.508 63.977 11.698 1.00 59. ATOM 320 CA ASN A 74 66.899 67.994 12.867 1.00 59. ATOM 320 CA	15	ATOM ATOM ATOM ATOM	279 CD2 LEU A 280 N TYR A 281 CA TYR A 282 C TYR A	69 70 70 70	54.687 57.642 58.696	65.522 62.392 61.726	6.120 8.132 8.897	1.00 37.17 1.00 39.01
ATOM 288 CE1 TYR A 70 61.792 59.957 8.267 1.00 42. ATOM 289 CE2 TYR A 70 61.274 58.190 10.309 1.00 41. ATOM 290 CZ TYR A 70 62.564 58.351 9.847 1.00 43. ATOM 291 OH TYR A 70 62.564 58.351 9.847 1.00 43. ATOM 292 N LYS A 71 60.057 62.793 10.582 1.00 48. ATOM 293 CA LYS A 71 60.980 63.806 11.069 1.00 52. ATOM 294 C LYS A 71 60.980 63.806 11.069 1.00 52. ATOM 295 O LYS A 71 62.343 63.205 11.258 1.00 54. ATOM 297 CG LYS A 71 62.343 63.205 11.258 1.00 54. ATOM 298 CD LYS A 71 60.466 64.499 12.359 1.00 54. ATOM 298 CD LYS A 71 59.964 63.608 13.478 1.00 56. ATOM 299 CE LYS A 71 59.964 63.608 13.478 1.00 56. ATOM 299 CE LYS A 71 59.964 63.608 13.478 1.00 56. ATOM 300 NZ LYS A 71 59.964 63.608 13.478 1.00 56. ATOM 300 NZ LYS A 71 59.964 63.608 13.478 1.00 56. ATOM 300 NZ LYS A 71 59.964 63.608 13.478 1.00 56. ATOM 301 N GLN A 72 63.230 63.514 10.306 1.00 55. ATOM 302 CA GLN A 72 64.616 63.821 10.317 1.00 57. ATOM 303 C GLN A 72 65.450 64.235 10.843 1.00 55. ATOM 304 O GLN A 72 65.450 64.235 10.843 1.00 55. ATOM 305 CB GLN A 72 65.450 64.235 10.843 1.00 58. ATOM 306 CG GLN A 72 66.361 61.951 8.881 1.00 59. ATOM 307 CD GLN A 72 66.361 61.951 8.881 1.00 59. ATOM 308 NEI GLN A 72 66.596 61.238 6.613 1.00 60. ATOM 309 NEZ GLN A 72 66.596 61.238 6.613 1.00 60. ATOM 309 NEZ GLN A 72 66.596 61.238 6.613 1.00 60. ATOM 310 N GLU A 73 65.903 65.918 12.992 1.00 58.4 ATOM 310 N GLU A 73 65.903 65.918 12.992 1.00 58.4 ATOM 310 C GLU A 73 65.903 65.918 12.992 1.00 58.4 ATOM 310 C GLU A 73 65.903 65.918 12.992 1.00 58.4 ATOM 312 C GLU A 73 65.903 65.993 12.992 1.00 58.4 ATOM 312 C GLU A 73 65.903 65.918 12.992 1.00 58.4 ATOM 313 CB GLU A 73 65.903 68.911 1.588 1.00 59. ATOM 310 CB GLU A 73 65.903 68.911 1.00 59. ATOM 312 C GLU A 73 65.903 65.918 12.992 1.00 58.4 ATOM 313 CB GLU A 73 65.903 65.918 12.992 1.00 59.4 ATOM 312 C G SAN A 74 65.859 67.193 12.548 1.00 59.6 ATOM 320 C A SSN A 74 65.859 67.993 11.698 1.00 66.2 ATOM 320 C A SSN A 74 65.859 67.993 11.698 1.00 59.0 ATOM 322 CG ASN A 74 65.860 68.574 16.283 1.00 60.0 ATOM 322 CG ASN	20	ATOM ATOM ATOM	284 CB TYR A 285 CG TYR A	70 70	59.352 60.490	60.618 59.832	8.067 8.721	1.00 43.81 1.00 41.37 1.00 41.66
25 ATOM 291 OH TYR A 70 63.594 57.643 10.399 1.00 43. ATOM 292 N LYS A 71 60.057 62.793 10.582 1.00 443. ATOM 293 CA LYS A 71 60.980 63.806 11.069 1.00 52. ATOM 294 C LYS A 71 62.343 63.205 11.258 1.00 54. ATOM 295 O LYS A 71 62.343 63.205 11.258 1.00 54. ATOM 296 CB LYS A 71 62.560 62.450 12.201 1.00 54. ATOM 297 CG LYS A 71 59.964 63.608 13.478 1.00 56. ATOM 298 CD LYS A 71 59.964 63.608 13.478 1.00 56. ATOM 299 CE LYS A 71 59.964 63.608 13.478 1.00 56. ATOM 299 CE LYS A 71 59.964 63.608 13.478 1.00 56. ATOM 300 NZ LYS A 71 59.964 63.608 13.478 1.00 56. ATOM 301 N GLN A 72 63.396 15.156 1.00 64. ATOM 302 CA GLN A 72 64.616 63.082 10.317 1.00 57. ATOM 303 C GLN A 72 65.450 64.235 10.843 1.00 58. ATOM 305 CB GLN A 72 65.382 65.341 10.304 1.00 58. ATOM 306 CG GLN A 72 66.409 60.910 7.782 1.00 59. ATOM 307 CD GLN A 72 66.596 61.238 6.613 1.00 59. ATOM 308 OE1 GLN A 72 66.596 61.238 6.613 1.00 59. ATOM 309 NE2 GLN A 72 66.596 61.238 6.613 1.00 59. ATOM 310 N GLU A 73 66.258 63.976 11.872 1.00 59. ATOM 310 N GLU A 73 66.258 63.976 11.872 1.00 59. ATOM 311 CA GLU A 73 66.258 63.976 11.872 1.00 59. ATOM 312 C GLU A 73 65.903 65.938 12.992 1.00 58. ATOM 313 O GLU A 73 66.258 63.976 11.872 1.00 59. ATOM 313 O GLU A 73 66.258 63.976 11.872 1.00 59. ATOM 314 CB GLU A 73 66.258 63.976 11.872 1.00 59. ATOM 315 CG GLU A 73 65.903 65.938 12.992 1.00 58. ATOM 316 CD GLU A 73 66.258 63.976 11.872 1.00 59. ATOM 317 OE1 GLU A 73 66.258 69.938 12.992 1.00 58. ATOM 318 OE2 GLU A 73 69.968 64.774 11.062 1.00 66. ATOM 319 N ASN A 74 66.469 67.994 12.587 1.00 57. ATOM 320 C ASN A 74 63.977 68.548 11.619 1.00 57. ATOM 321 C ASN A 74 66.469 67.994 12.587 1.00 57. ATOM 322 C ASN A 74 66.309 69.397 11.698 1.00 57. ATOM 323 CB ASN A 74 66.469 67.994 12.587 1.00 57. ATOM 324 CG ASN A 74 66.409 68.397 11.698 1.00 57. ATOM 325 ODI ASN A 74 66.409 69.397 11.698 1.00 57. ATOM 326 CA ASN A 74 66.5015 69.039 13.938 1.00 57.66. ATOM 327 N ASN A 74 66.406 66.222 9.570 1.00 48.0 ATOM 328 CA ASN A 75 62.360 67.397 9.195 1.00 48.1 ATOM 329 C ASN A 75		ATOM ATOM	287 CD2 TYR A 288 CE1 TYR A 289 CE2 TYR A	70 70 70	61.792 61.274 62.826	59.957 58.190 59.218	8.267 10.309 8.823	1.00 42.62 1.00 41.91 1.00 43.07
ATOM 295 C LYS A 71 62.343 63.205 11.258 1.00 54. ATOM 295 C LYS A 71 62.540 62.450 62.450 12.201 1.00 54. ATOM 296 CB LYS A 71 59.964 63.608 13.478 1.00 56. ATOM 297 CG LYS A 71 59.964 63.608 13.478 1.00 56. ATOM 299 CD LYS A 71 59.964 63.608 13.478 1.00 56. ATOM 299 CE LYS A 71 58.518 63.648 15.658 1.00 63. ATOM 300 NZ LYS A 71 57.109 63.396 11.6516 1.00 64. ATOM 301 N GLN A 72 63.230 63.514 10.306 1.00 57. ATOM 302 CA GLN A 72 64.616 63.082 10.317 1.00 57. ATOM 303 C GLN A 72 65.450 64.235 10.843 10.055. ATOM 305 CB GLN A 72 65.450 64.235 10.843 10.05 58. ATOM 306 CG GLN A 72 65.366 64.235 10.843 1.00 58. ATOM 307 CD GLN A 72 66.361 61.951 8.881 1.00 59. ATOM 308 OEI GLN A 72 66.361 61.951 8.881 1.00 59. ATOM 309 NEZ GLN A 72 66.596 61.238 6.613 1.00 60. ATOM 310 N GLU A 73 66.258 63.976 11.872 1.00 59. ATOM 311 CA GLU A 73 66.258 63.976 11.872 1.00 59. ATOM 312 C GLU A 73 67.020 65.043 12.493 1.00 59. ATOM 313 O GLU A 73 67.903 65.938 12.992 1.00 58. ATOM 313 O GLU A 73 67.904 65.471 11.00 58. ATOM 313 O GLU A 73 67.904 65.973 8.986 1.00 59. ATOM 313 CB GLU A 73 67.904 65.973 8.986 1.00 59. ATOM 313 CB GLU A 73 67.904 65.973 8.986 1.00 59. ATOM 313 CB GLU A 73 67.904 65.973 8.986 1.00 59. ATOM 313 CB GLU A 73 67.904 65.973 8.986 1.00 59. ATOM 315 CG GLU A 73 67.904 65.973 8.986 1.00 59. ATOM 316 CD GLU A 73 67.904 65.973 8.986 1.00 59. ATOM 317 OEI GLU A 73 67.906 65.470 13.791 1.00 58. ATOM 318 OEZ GLU A 73 67.906 65.973 8.986 1.00 66.2 ATOM 320 CA ASN A 74 65.859 67.193 12.548 1.00 59. ATOM 321 C ASN A 74 65.859 67.193 12.548 1.00 57. ATOM 322 C ASN A 74 65.859 67.193 12.548 1.00 59. ATOM 323 CB ASN A 74 65.359 68.391 15.263 1.00 59. ATOM 324 CG ASN A 74 65.359 68.391 15.263 1.00 59. ATOM 325 ODI ASN A 74 66.460 68.574 16.283 1.00 59. ATOM 320 C ASN A 75 63.356 66.22 9.977 11.00 50.2 ATOM 330 O ASN A 75 63.356 66.22 9.977 11.00 50.2 ATOM 330 O ASN A 75 63.558 68.319 9.274 1.00 50.2 ATOM 331 ODI ASN A 75 65.573 69.129 8.049 1.00 50.2	25	ATOM ATOM ATOM	291 OH TYR A 292 N LYS A 293 CA LYS A	70 71	63.594 60.057	57.643 62.793	10.399 10.582	1.00 43.67 1.00 43.42 1.00 48.84 1.00 52.37
ATOM 299 CE LYS A 71 58.518 63.4648 15.658 1.00 63. ATOM 300 NZ LYS A 71 57.109 63.396 15.156 1.00 64. ATOM 301 N GLN A 72 63.230 63.514 10.306 1.00 56. ATOM 302 CA GLN A 72 64.616 63.082 10.317 1.00 57. ATOM 303 C GLN A 72 65.450 64.235 10.843 1.00 58. ATOM 304 O GLN A 72 65.382 65.341 10.304 1.00 58. ATOM 305 CB GLN A 72 65.073 62.737 8.905 1.00 57. ATOM 306 CG GLN A 72 66.361 61.951 8.881 1.00 59. ATOM 307 CD GLN A 72 66.361 61.951 8.881 1.00 59. ATOM 308 OE1 GLN A 72 66.596 61.238 6.613 1.00 60. ATOM 309 NE2 GLN A 72 66.596 61.238 6.613 1.00 60. ATOM 310 N GLU A 73 66.258 63.976 11.872 1.00 58. ATOM 311 CA GLU A 73 66.258 63.976 11.872 1.00 58. ATOM 312 C GLU A 73 67.020 65.043 12.493 1.00 58. ATOM 313 O GLU A 73 65.903 65.938 12.493 1.00 59. ATOM 314 CB GLU A 73 67.020 65.043 12.493 1.00 59. ATOM 315 CG GLU A 73 67.020 65.938 12.493 1.00 59. ATOM 316 CD GLU A 73 67.020 65.938 12.493 1.00 59. ATOM 317 OE1 GLU A 73 65.904 65.718 11.481 1.00 59. ATOM 318 OE2 GLU A 73 67.963 65.718 11.481 1.00 59. ATOM 319 N ASN A 74 65.898 64.988 9.647 1.00 64.6 ATOM 319 N ASN A 74 65.899 67.193 12.548 1.00 57.4 ATOM 319 N ASN A 74 65.899 67.193 12.548 1.00 57.4 ATOM 320 CA ASN A 74 63.997 68.548 11.619 1.00 54.8 ATOM 322 O ASN A 74 65.399 68.391 15.2563 1.00 59. ATOM 325 ODI ASN A 74 65.399 68.391 15.2563 1.00 59. ATOM 326 ND ASN A 74 65.399 68.391 15.263 1.00 59. ATOM 327 N ASN A 74 65.399 68.391 15.263 1.00 59. ATOM 328 CA ASN A 74 65.399 68.391 15.263 1.00 59. ATOM 329 C ASN A 74 65.399 68.391 15.263 1.00 59. ATOM 329 C ASN A 74 65.399 68.391 15.263 1.00 59. ATOM 320 CA ASN A 74 65.399 68.391 15.263 1.00 59. ATOM 320 CA ASN A 74 65.399 68.391 15.2563 1.00 65. ATOM 320 CA ASN A 75 62.425 66.222 9.570 1.00 48.0 ATOM 320 CA ASN A 75 62.425 66.222 9.570 1.00 48.0 ATOM 320 CA ASN A 75 62.425 66.222 9.570 1.00 48.0 ATOM 331 CB ASN A 75 62.425 66.222 9.570 1.00 48.0 ATOM 332 CB ASN A 75 62.425 66.222 9.570 1.00 48.0 ATOM 333 ODI ASN A 75 62.425 66.222 9.570 1.00 50.2 ATOM 333 ODI ASN A 75 62.446 70.282 7.691 1.00 50.2	30	ATOM ATOM ATOM	295 O LYS A 296 CB LYS A 297 CG LYS A	71 71 71	62.560 60.496 59.964	62.450 64.499 63.608	11.258 12.201 12.359 13.478	1.00 54.20 1.00 54.67 1.00 53.08 1.00 56.42
ATOM 303 C GLN A 72 65.450 64.235 10.843 1.00 58. ATOM 304 O GLN A 72 65.382 65.341 10.304 1.00 58. ATOM 305 CB GLN A 72 65.073 62.737 8.905 1.00 57. ATOM 306 CG GLN A 72 66.361 61.951 8.881 1.00 59. ATOM 307 CD GLN A 72 66.409 60.910 7.782 1.00 59. ATOM 308 OE1 GLN A 72 66.596 61.238 6.613 1.00 60. ATOM 309 NE2 GLN A 72 66.596 61.238 6.613 1.00 60. ATOM 310 N GLU A 73 66.258 63.976 11.872 1.00 59. ATOM 311 CA GLU A 73 65.903 65.938 12.493 1.00 59. ATOM 312 C GLU A 73 65.903 65.938 12.992 1.00 58. ATOM 313 O GLU A 73 65.903 65.938 12.992 1.00 58. ATOM 314 CB GLU A 73 65.064 65.470 13.791 1.00 58. ATOM 315 CG GLU A 73 67.963 65.718 11.481 1.00 59. ATOM 316 CD GLU A 73 69.086 64.774 11.062 1.00 62. ATOM 317 OE1 GLU A 73 69.598 64.988 9.647 1.00 64.6 ATOM 318 OE2 GLU A 73 70.406 64.154 9.195 1.00 66.2 ATOM 319 N ASN A 74 65.859 67.193 12.548 1.00 57.4 ATOM 320 CA ASN A 74 65.859 67.193 12.548 1.00 57.4 ATOM 321 C ASN A 74 63.092 69.397 11.698 1.00 55.68 ATOM 321 C ASN A 74 63.092 69.397 11.698 1.00 57.4 ATOM 322 O ASN A 74 63.092 69.397 11.698 1.00 57.6 ATOM 323 CB ASN A 74 65.399 68.391 15.263 1.00 59.0 ATOM 326 ND2 ASN A 74 66.429 67.702 15.356 1.00 59.0 ATOM 327 N ASN A 74 66.429 67.702 15.356 1.00 59.0 ATOM 328 CA ASN A 74 66.429 67.702 15.356 1.00 59.0 ATOM 329 C ASN A 74 66.429 67.702 15.356 1.00 59.0 ATOM 320 CA ASN A 74 66.429 67.702 15.356 1.00 59.0 ATOM 322 CB ASN A 74 66.429 67.702 15.356 1.00 59.0 ATOM 325 OD1 ASN A 74 66.429 67.702 15.356 1.00 59.0 ATOM 326 ND2 ASN A 74 66.429 67.702 15.356 1.00 59.0 ATOM 327 N ASN A 75 66.358 68.319 9.274 1.00 50.2 ATOM 330 O ASN A 75 66.358 68.319 9.274 1.00 50.2 ATOM 331 CB ASN A 75 66.366 67.397 9.195 1.00 48.0 ATOM 332 CG ASN A 75 66.5573 69.129 8.049 1.00 50.2 ATOM 333 OD1 ASN A 75 66.5573 69.129 8.049 1.00 50.2	35	ATOM ATOM ATOM	299 CE LYS A 300 NZ LYS A 301 N GLN A	71 71 72	58.518 57.109 63.230	63.648 63.396 63.514	15.658 15.156 10.306	1.00 63.37 1.00 64.08 1.00 56.38
ATOM 308 OE1 GLN A 72 66.596 61.238 6.613 1.00 60 ATOM 309 NE2 GLN A 72 66.273 59.651 8.160 1.00 59 ATOM 311 N GLU A 73 66.258 63.976 11.872 1.00 58.8 ATOM 311 CA GLU A 73 66.258 63.976 11.872 1.00 58.8 ATOM 312 C GLU A 73 65.903 65.938 12.992 1.00 58.8 ATOM 313 O GLU A 73 65.903 65.938 12.992 1.00 58.8 ATOM 314 CB GLU A 73 67.963 65.718 11.481 1.00 59 ATOM 315 CG GLU A 73 67.963 65.718 11.481 1.00 59 ATOM 316 CD GLU A 73 69.086 64.774 11.062 1.00 62.3 ATOM 317 OE1 GLU A 73 69.598 64.988 9.647 1.00 64.6 ATOM 317 OE1 GLU A 73 69.204 65.973 8.986 1.00 66.2 ATOM 319 N ASN A 74 65.859 67.193 12.548 1.00 57.4 ATOM 320 CA ASN A 74 65.859 67.193 12.548 1.00 57.4 ATOM 321 C ASN A 74 64.689 67.994 12.867 1.00 56.8 ATOM 322 O ASN A 74 63.977 68.548 11.619 1.00 54.8 ATOM 323 CB ASN A 74 65.399 68.391 15.263 1.00 59.0 ATOM 324 CG ASN A 74 65.399 68.391 15.263 1.00 59.0 ATOM 325 OD1 ASN A 74 65.399 68.391 15.263 1.00 59.0 ATOM 326 ND2 ASN A 74 66.429 67.702 15.356 1.00 61.5 ATOM 327 N ASN A 74 66.429 67.702 15.356 1.00 61.5 ATOM 328 CA ASN A 75 66.358 68.319 9.274 1.00 50.3 ATOM 329 C ASN A 75 64.330 68.016 10.462 1.00 52.2 ATOM 331 CB ASN A 75 64.330 68.016 10.462 1.00 52.2 ATOM 332 CG ASN A 75 62.360 67.397 9.195 1.00 48.1 ATOM 333 OD1 ASN A 75 66.440 68.186 8.027 1.00 50.3 ATOM 332 CG ASN A 75 66.573 69.129 8.049 1.00 50.2 ATOM 333 OD1 ASN A 75 65.573 69.129 8.049 1.00 50.2 ATOM 333 OD1 ASN A 75 65.573 69.129 8.049 1.00 50.2	40	ATOM ATOM ATOM	303 C GLN A 304 O GLN A 305 CB GLN A 306 CG GLN A 307 CD GLN A	72 72 72 72	65.450 65.382 65.073 66.361	64.235 65.341 62.737 61.951	10.843 10.304 8.905 8.881	1.00 58.19 1.00 58.25 1.00 57.62 1.00 59.06
ATOM 313 O GLU A 73 65.064 65.470 13.791 1.00 58.6 ATOM 314 CB GLU A 73 67.963 65.718 11.481 1.00 59.7 ATOM 315 CG GLU A 73 69.086 64.774 11.062 1.00 62.3 ATOM 316 CD GLU A 73 69.598 64.988 9.647 1.00 64.6 ATOM 317 OE1 GLU A 73 69.204 65.973 8.986 1.00 66.2 ATOM 318 OE2 GLU A 73 70.406 64.154 9.195 1.00 66.6 ATOM 319 N ASN A 74 65.859 67.193 12.548 1.00 57.4 ATOM 320 CA ASN A 74 64.689 67.994 12.867 1.00 56.8 ATOM 321 C ASN A 74 63.977 68.548 11.619 1.00 54.8 ATOM 322 O ASN A 74 63.977 68.548 11.619 1.00 54.8 ATOM 322 O ASN A 74 63.977 68.548 11.619 1.00 55.0 ATOM 323 CB ASN A 74 65.015 69.039 13.938 1.00 57.6 ATOM 324 CG ASN A 74 65.399 68.391 15.263 1.00 59.0 ATOM 325 OD1 ASN A 74 66.429 67.702 15.356 1.00 61.5 ATOM 326 ND2 ASN A 74 66.429 67.702 15.356 1.00 61.5 ATOM 328 CA ASN A 75 64.330 68.016 10.462 1.00 52.2 ATOM 329 C ASN A 75 64.330 68.016 10.462 1.00 52.2 ATOM 329 C ASN A 75 62.360 67.397 9.195 1.00 48.0 ATOM 329 C ASN A 75 62.360 67.397 9.195 1.00 48.0 ATOM 329 C ASN A 75 62.425 66.222 9.570 1.00 48.0 ATOM 331 CB ASN A 75 62.425 66.222 9.570 1.00 48.0 ATOM 332 CG ASN A 75 62.425 66.222 9.570 1.00 48.0 ATOM 332 CG ASN A 75 62.425 66.222 9.570 1.00 48.0 ATOM 333 OD1 ASN A 75 65.573 69.129 8.049 1.00 50.2 ATOM 333 OD1 ASN A 75 65.573 69.129 8.049 1.00 50.2 ATOM 333 OD1 ASN A 75 65.573 69.129 8.049 1.00 50.2 ATOM 333 OD1 ASN A 75 65.446 70.282 7.691 1.00 51.4	45	ATOM ATOM ATOM	309 NE2 GLN A 310 N GLU A 311 CA GLU A	72 73 73	66.596 66.273 66.258 67.020	61.238 59.651 63.976 65.043	6.613 8.160 11.872 12.493	1.00 60.39 1.00 59.37 1.00 58.85 1.00 59.44
ATOM 318 OE2 GLU A 73 70.406 64.154 9.195 1.00 66.6 ATOM 320 CA ASN A 74 65.859 67.193 12.548 1.00 57.4 ATOM 321 C ASN A 74 64.689 67.994 12.867 1.00 56.8 ATOM 322 O ASN A 74 63.977 68.548 11.619 1.00 54.8 ATOM 323 CB ASN A 74 65.015 69.039 13.938 1.00 57.6 ATOM 324 CG ASN A 74 65.399 68.391 15.263 1.00 57.6 ATOM 325 OD1 ASN A 74 66.429 67.702 15.356 1.00 61.5 ATOM 327 N ASN A 74 66.429 67.702 15.356 1.00 61.5 ATOM 328 CA ASN A 75 64.330 68.016 10.462 1.00 52.2 ATOM 329 C ASN A 75 64.330 68.016 10.462 1.00 52.2 ATOM 330 O ASN A 75 62.360 67.397 9.195 1.00 48.1 ATOM 331 CB ASN A 75 62.425 66.222 9.570 1.00 48.0 ATOM 332 CG ASN A 75 62.425 66.222 9.570 1.00 48.0 ATOM 332 CG ASN A 75 64.410 68.186 8.027 1.00 50.2 ATOM 333 OD1 ASN A 75 65.573 69.129 8.049 1.00 50.2 ATOM 333 OD1 ASN A 75 65.573 69.129 8.049 1.00 50.2 ATOM 333 OD1 ASN A 75 65.573 69.129 8.049 1.00 50.2 ATOM 333 OD1 ASN A 75 65.573 69.129 8.049 1.00 50.2 ATOM 333 OD1 ASN A 75 65.446 70.282 7.691 1.00 51.4	50	ATOM ATOM ATOM	313 O GLU A 314 CB GLU A 315 CG GLU A 316 CD GLU A	73 73 73 73	65.064 67.963 69.086 69.598	65.470 65.718 64.774 64.988	13.791 11.481 11.062 9.647	1.00 58.69 1.00 59.71 1.00 62.37 1.00 64.62
ATOM ATOM 324 CG ASN A 74 65.015 69.039 13.938 1.00 57.6 ATOM 325 OD1 ASN A 74 65.399 68.391 15.263 1.00 59.0 ATOM 325 OD1 ASN A 74 66.429 67.702 15.356 1.00 61.5 ATOM 327 N ASN A 75 64.560 68.574 16.283 1.00 60.0 ATOM 328 CA ASN A 75 64.330 68.016 10.462 1.00 52.2 ATOM 329 C ASN A 75 63.558 68.319 9.274 1.00 50.3 ATOM 330 O ASN A 75 62.360 67.397 9.195 1.00 48.1 ATOM 331 CB ASN A 75 62.425 66.222 9.570 1.00 48.0 ATOM 332 CG ASN A 75 64.410 68.186 8.027 1.00 50.2 ATOM 333 OD1 ASN A 75 65.573 69.129 8.049 1.00 50.2 ATOM 333 OD1 ASN A 75 65.573 69.129 8.049 1.00 50.2	55	ATOM ATOM ATOM ATOM ATOM	318 OE2 GLU A 319 N ASN A 320 CA ASN A 321 C ASN A 322 O ASN A	73 74 74 74 74	70.406 65.859 64.689 63.977 63.092	64.154 67.193 67.994 68.548	9.195 12.548 12.867 11.619	1.00 66.20 1.00 66.62 1.00 57.47 1.00 56.86 1.00 54.85 1.00 55.01
ATOM 329 C ASN A 75 63.558 68.319 9.274 1.00 50.3 ATOM 329 C ASN A 75 62.360 67.397 9.195 1.00 48.1 ATOM 330 O ASN A 75 62.425 66.222 9.570 1.00 48.0 ATOM 331 CB ASN A 75 64.410 68.186 8.027 1.00 50.2 ATOM 332 CG ASN A 75 65.573 69.129 8.049 1.00 50.2 ATOM 333 OD1 ASN A 75 65.446 70.282 7.691 1.00 51.4	60	ATOM ATOM ATOM ATOM	324 CG ASN A 325 OD1 ASN A 326 ND2 ASN A 327 N ASN A	74 74 74 75	65.399 66.429 64.560 64.330	68.391 67.702 68.574	13.938 15.263 15.356 16.283	1.00 57.63 1.00 59.00 1.00 61.58 1.00 60.07 1.00 52.29
ATOM 333 OD1 ASN A 75 65.446 70.282 7.691 1.00 51.4	65	ATOM ATOM ATOM	329 C ASN A 330 O ASN A 331 CB ASN A	75 75 75	62.360 62.425 64.410	68.319 67.397 66.222 68.186	9.274 9.195 9.570 8.027	1.00 50.31 1.00 48.13 1.00 48.00 1.00 50.26
ATOM 335 N ILE A 76 61.246 67.953 8.750 1.00 44.9	70	ATOM ATOM ATOM	333 OD1 ASN A 334 ND2 ASN A 335 N ILE A	75 75 76	65.446 66.697 61.246	70.282 68.661 67.953	7.691 8.542 8.750	1.00 50.23 1.00 51.42 1.00 50.94 1.00 44.92 1.00 42.61

	ATOM ATOM ATOM	337 338 339	C O CB	ILE A ILE A ILE A	76 76 76	60.024 60.026 58.822	66.853 67.733 67.869	7.052 6.247 9.015	1.00 39.17 1.00 38.33 1.00 42.75
5	ATOM ATOM ATOM ATOM	340 341 342 343	CG1 CG2 CD1 N	ILE A	76 76 76 77	58.971 57.605 57.881 60.002	68.180 67.001 69.115 65.581	10.512 8.788 11.061 6.731	1.00 44.18 1.00 43.04 1.00 46.10 1.00 37.03
10	ATOM ATOM ATOM ATOM	344 345 346 347	CA C O CB	LEU A LEU A LEU A	77 77 77 77	60.044 58.709 58.071 61.059	65.121 64.557 63.900 63.991	5.359 4.990 5.786 5.200	1.00 35.58 1.00 34.01 1.00 33.20 1.00 34.83
15	ATOM ATOM ATOM ATOM	348 349 350 351	CG CD1	LEU A LEU A LEU A VAL A	77 77 77 78	62.442 63.355 62.997 58.283	64.220 63.054 65.543 64.827	5.769 5.417 5.208 3.775	1.00 35.71 1.00 36.23 1.00 37.79 1.00 32.73
13	ATOM ATOM ATOM	352 353 354	CA C O CB	VAL A VAL A VAL A VAL A	78 78 78 78	57.109 57.565 58.464 56.074	64.165 63.084 63.296 65.137	3.268 2.282 1.464 2.673	1.00 32.11 1.00 31.94 1.00 29.80 1.00 33.08
20	ATOM ATOM ATOM ATOM	355 356 357 358	CG1 CG2 N	VAL A VAL A PHE A	78 78 79	56.620 54.851 56.976	66.060 64.359 61.907	1.620 2.110 2.459	1.00 34.71 1.00 34.03 1.00 30.10
25	ATOM ATOM ATOM ATOM	359 360 361 362	CA C O CB	PHE A PHE A PHE A	79 79 79 79	57.167 55.902 54.796 57.478	60.723 60.331 60.439 59.542	1.632 0.855 1.369 2.541	1.00 30.28 1.00 29.50 1.00 28.83 1.00 30.42
30	MOTA MOTA MOTA	363 364 365 366	CD2	PHE A PHE A PHE A	79 79 79 79	58.882 59.339 59.753 60.651	59.521 60.474 58.553 60.449	3.032 3.937 2.591 4.378	1.00 30.64 1.00 30.69 1.00 31.60 1.00 32.56
	ATOM ATOM ATOM ATOM	367 368 369 370	CE2 CZ N CA	PHE A PHE A ASN A ASN A	79 79 80 80	61.078 61.514 56.095 55.053	58.533 59.483 59.856 59.271	3.040 3.931 -0.370 -1.194	1.00 31.97 1.00 31.51 1.00 28.48 1.00 28.45
35	ATOM ATOM ATOM ATOM	371 372 373 374	C O CB CG	ASN A ASN A ASN A	80 80 80 80	55.145 56.177 55.280 54.274	57.756 57.195 59.664 59.019	-1.039 -1.298 -2.656 -3.593	1.00 28.68 1.00 29.34 1.00 28.49 1.00 28.68
40	ATOM ATOM ATOM	375 376 377	OD1 ND2 N	ASN A ASN A ALA A	80 80 81	54.264 53.440 54.108	57.785 59.845 57.081 55.647	-3.747 -4.238 -0.575 -0.280	1.00 31.70 1.00 26.72 1.00 28.87 1.00 29.20
45	ATOM ATOM ATOM ATOM	378 379 380 381	CA C O CB	ALA A ALA A ALA A	81 81 81	54.221 54.367 55.068 53.055	54.692 53.667 55.226	-1.486 -1.391 0.529	1.00 30.47 1.00 28.22 1.00 29.86
	ATOM ATOM ATOM ATOM	382 383 384 385	N CA C O	GLU A GLU A GLU A	82 82 82 82	53.692 53.690 55.085 55.584	55.009 54.163 54.085 53.005	-2.584 -3.765 -4.380 -4.642	1.00 30.69 1.00 32.90 1.00 32.70 1.00 33.55
50	ATOM ATOM ATOM ATOM	386 387 388 389	CB CG CD OE1	GLU A GLU A GLU A	82 82 82 82	52.762 51.904 51.966 51.733	54.778 53.921 52.395 51.877	-4.799 -5.750 -5.602 -4.479	1.00 34.29 1.00 39.11 1.00 44.08 1.00 44.47
55	ATOM ATOM ATOM ATOM	390 391 392 393		GLU A TYR A TYR A TYR A	82 83 83 83	52.146 55.711 56.988 58.174	51.715 55.239 55.343 55.575	-6.659 -4.577 -5.293 -4.375	1.00 45.29 1.00 32.46 1.00 31.80 1.00 32.14
60	ATOM ATOM ATOM	394 395 396	O CB CG	TYR A TYR A TYR A	83 83 83	59.315 56.894 55.736	55.439 56.474 56.289	-4.779 -6.341 -7.262	1.00 31.65 1.00 30.74 1.00 27.96
	ATOM ATOM ATOM ATOM	397 398 399 400	CD2 CE1 CE2	TYR A TYR A TYR A TYR A	83 83 83	55.723 54.612 54.640 53.510	55.245 57.127 55.039 56.937	-8.168 -7.189 -9.025 -8.014	1.00 26.86 1.00 30.33 1.00 30.17 1.00 30.63
65	ATOM ATOM ATOM ATOM	401 402 403 404	CZ OH N CA	TYR A TYR A GLY A GLY A	83 83 84 84	53.532 52.481 57.916 58.994	55.881 55.683 55.975 56.133	-8.934 -9.777 -3.135 -2.186	1.00 32.85 1.00 32.80 1.00 32.26 1.00 31.32
70	ATOM ATOM	405 406	C O	GLY A	84 84	59.847 60.834	57.373 57.521	-2.335 -1.613	1.00 31.68 1.00 31.73

	ATOM	40	7 N	ASN .	A 85	59.498	8 58.278	-3.245	5 1.00 31.53
	ATOM	40	8 C			60.243			
	ATOM	40	9 C	ASN .		59.864			
	ATOM	41		ASN A	A 85	58.797			1.00 32.48
	5 ATOM	41				60.048	8 60.160		
	ATOM	41:				58.654		-4.935	1.00 30.02
	ATOM	41		O1 ASN		57.69 <i>6</i>			
	ATOM	414			_	58.543			1.00 30.08
10	MOTA	415		SER A		60.738			1.00 33.04
10	ATOM ATOM	416 417				60.474		-0.704	
	ATOM	418		SER A		61.111		-0.858	
	MOTA	419		SER A SER A		61.992		-1.699	
	ATOM	420				60.946		0.578	
15		421		SER A		62.361 60.633		0.669	
	ATOM	422				61.155		-0.059	
	ATOM	423		SER A	_	61.047		-0.090 1.265	
	ATOM	424		SER A		60.455		2.173	1.00 38.73
	ATOM	425	СВ		-	60.383		-1.079	1.00 37.89 1.00 37.51
20		426		SER A		59.126		-1.378	1.00 37.31
	ATOM	427		VAL A	88	61.589		1.409	1.00 39.45
	ATOM	428				61.470	68.393	2.679	1.00 41.20
	ATOM	429		VAL A		60.213	69.269	2.720	1.00 41.11
25	ATOM	430	-	VAL A		59.995	70.168	1.903	1.00 41.19
23	ATOM ATOM	431	_			62.803	69.144	3.105	1.00 42.08
	ATOM	432 433				63.609		1.901	1.00 44.39
	ATOM	433	CG:			62.484	70.266	4.121	1.00 42.80
	ATOM	. 435	CA	PHE A PHE A		59.354	68.923	3.668	1.00 42.02
30	ATOM	436	C	PHE A		58.158	69.691	3.946	1.00 42.61
	ATOM	437	Ö	PHE A		58.515 58.174	70.913 72.006	4.740	1.00 42.65
	ATOM	438	ČВ	PHE A	89	57.175	68.901	4.372	1.00 40.97
	ATOM	439	CG	PHE A	89	55.908	69.650	4.774 5.053	1.00 43.24
	ATOM	440	CD:		89	55.192	70.213	4.019	1.00 45.25 1.00 48.71
35	ATOM	441	CD2		89	55.450	69.813	6.342	1.00 47.88
	ATOM	442	CE	l PHE A	89	54.028	70.900	4.266	1.00 50.50
	ATOM	443	CE2	PHE A	89	54.292	70.492	6.594	1.00 48.14
	ATOM	444	CZ	PHE A	89	53.578	71.034	5.562	1.00 50.14
40	ATOM	445	N	LEU A	90	59.219	70.716	5.843	1.00 44.35
40	ATOM	446		LEU A	90	59.602	71.839	6.662	1.00 46.14
	ATOM	447	C	LEU A	90	61.058	71.751	7.079	1.00 46.98
	ATOM ATOM	448 449	0	LEU A	90	61.460	70.856	7.826	1.00 45.46
	ATOM	450	CB CG	LEU A LEU A	90 90	58.679	71.910	7.874	1.00 46.70
45	ATOM	451	CD1		90	58.692 57.850	73.226	8.634	1.00 47.52
	ATOM	452		LEU A	90	60.091	73.069 73.614	9.878	1.00 48.98
	ATOM	453	N	GLU A	91	61.852	73.614	9.015	1.00 48.42
	ATOM	454	CA	GLU A	91	63.274	72.711	6.570	1.00 49.09
	ATOM	455	С	GLU A	91	63.458	72.982	6.877 8.338	1.00 51.12
50	ATOM	456	0	GLU A	91	62.770	73.830	8.903	1.00 52.09 1.00 51.30
•	ATOM	457	СВ	GLU A	91	63.988	73.808	6.125	1.00 51.65
	ATOM	458	CG	GLU A	91	64.529	73.406	4.785	1.00 54.17
	ATOM	459	CD	GLU A	91	64.541	74.582	3.827	1.00 57.08
	ATOM	460		GLU A	91	63.540	75.332	3.832	1.00 58.58
55	ATOM	461	OE2		91	65.527	74.747	3.080	1.00 57.71
	ATOM	462	N	ASN A	92	64.419	72.274	8.920	1.00 54.09
	ATOM ATOM	463	CA	ASN A	92	64.758	72.390	10.323	1.00 55.48
	ATOM	464	C	ASN A	92	65.158	73.822	10.655	1.00 56.47
60	ATOM	465 466	0	ASN A	92	65.072	74.238	11.798	1.00 56.53
00	ATOM	467	CB	ASN A	92	65.891	71.404	10.679	1.00 56.01
	ATOM	468	CG OD1	ASN A	92	67.215	71.747	9.995	1.00 56.92
	ATOM	468		ASN A ASN A	92 92	67.374	72.851	9.475	1.00 58.85
	ATOM	470	ND2	SER A	92 93	68.167	70.801	9.994	1.00 55.37
65	ATOM	471	CA	SER A	93	65.580 65.998	74.568	9.641	1.00 57.67
	ATOM	472	C	SER A	93	64.889	75.956 77.022	9.812	1.00 59.12
	ATOM	473	Õ	SER A	93	65.141	77.022 78.116	9.927	1.00 59.80
	ATOM	474	ČВ	SER A	93	66.904	76.116	10.453	1.00 59.65
	ATOM	475	ŌĠ	SER A	93	66.789	75.443	8.639 7.558	1.00 59.16 1.00 60.69
70	ATOM	476	N	THR A	94	63.683	76.718	9.452	1.00 60.69
									1.00 00.44

	ATOM	477	CA	MHD	7	0.4	62 600	77 720	0 270	1 00	61 40
			CA	THR		94	62.608	77.720	9.370		61.40
	MOTA	478	С	THR	Α	94	62.407	78.609	10.610		61.76
	MOTA	479	0	THR	Α	94	62.315	79.829	10.506	1.00	61.08
	ATOM	480	CB	THR	Α	94	61.272	77.027	9.052		61.66
5	ATOM	481	OG1			94	61.411	76.211	7.881		63.17
_		482									
	ATOM		CG2			94	60.204	78.042	8.677		62.07
	ATOM	483	N	PHE		95	62.318	77.995	11.781		62.61
	ATOM	484	CA	PHE	Α	95	62.044	78.753	12.990	1.00	63.25
	ATOM	485	С	PHE	Α	95	63.298	79.067	13.829		64.05
10	ATOM	486	ō	PHE		95	63.249	79.072	15.050		63.10
	ATOM	487	СВ	PHE		95	60.982	78.015			
									13.811		63.31
	MOTA	488	CG	PHE		95	59.767	77.614	13.009		61.93
	ATOM	489		PHE		95	58.862	78.565	12.582		60.41
	ATOM	490	CD2	PHE	Α	95	59.536	76.282	12.687	1.00	60.39
15	ATOM	491	CE1	PHE	Α	95	57.746	78.197	11.854	1.00	
	ATOM	492	CE2			95	58.433	75.917	11.967		59.98
	ATOM	493	CZ	PHE		95	57.531	76.881	11.544		59.56
	ATOM	494	N	ASP	Α	96	64.418	79.345	13.163	1.00	65.57
	ATOM	495	CA	ASP	Α	96	65.651	79.720	13.874	1.00	66.85
20	ATOM	496	С	ASP	Α	96	65.436	80.979	14.732	1.00	67.10
	ATOM	497	ō	ASP		96	65.902	81.043	15.863	1.00	
	ATOM	498	СВ	ASP		96		79.952	12.899		
							66.821				67.18
	ATOM	499	CG	ASP		96	67.442	78.649	12.383		68.19
	ATOM	500	OD1	ASP	Α	96	66.948	77.554	12.742		69.92
25	ATOM	501	OD2	ASP	Α	96	68.432	78.630	11.613	1.00	68.66
	ATOM	502	N	GLU	Α	97	64.725	81.968	14.197		67.56
	ATOM	503	CA	GLU		97	64.459	83.209	14.936	1 00	67.97
	ATOM	504				97					
			C	GLU			63.127	83.189	15.714	1.00	
	ATOM	505	0	GLU		97	62.552	84.234	16.000		67.78
30	ATOM	506	CB	GLU	Α	97	64.515	84.432	13.994	1.00	67.97
	ATOM	507	CG	GLU	Α	97	65.920	84.765	13.490	1.00	68.74
	ATOM	508	CD	GLU	Α	97	66.349	86.191	13.828		69.30
	ATOM	509	OE1	GLU		97	66.456	86.505	15.033		68.09
2.5	ATOM	510	OE2			97	66.582	87.001	12.895	1.00	
35	ATOM	511	N	PHE		98	62.648	82.005	16.066	1.00	67.34
	ATOM	512	CA	PHE	Α	98	61.422	81.898	16.839	1.00	67.25
	ATOM	513	С	PHE	Α	98	61.657	82.331	18.272	1.00	66.90
	ATOM	514	0	PHE		98	60.790	82.911	18.906	1.00	
	ATOM	515	ČВ	PHE		98	60.933	80.464	16.857	1.00	
40		516									
40	ATOM		CG	PHE		98	59.548	80.311	17.401		67.61
	ATOM	517	CD1	PHE	A	98	58.468	80.818	16.715	1.00	68.05
	MOTA	518	CD2	PHE	Α	98	59.325	79.663	18.597	1.00	67.98
	ATOM	519	CE1	PHE	Α	98	57.190	80.674	17.211	1.00	68.39
	ATOM	520	CE2	PHE		98	58.046	79.515	19.092		67.80
45	ATOM	521	CZ								
43				PHE		98	56.983	80.021	18.399		67.93
	MOTA	522	N	GLY		99	62.833	82.003	18.788		66.78
	MOTA	523	CA	GLY .	Α	99	63.204	82.374	20.139	1.00	66.53
	MOTA	524	С	GLY .	Α	99	62.856	81.297	21.133	1.00	66.11
	ATOM	525	0	GLY .	Α	99	63.455	81.211	22.201	1.00	66.86
50	ATOM	526	N	HIS			61.885	80.466	20.787		65.36
•	ATOM	527	CA	HIS .			61.447	79.418	21.693		
											64.86
	ATOM	528	C	HIS.			61.783	78.023	21.161		64.00
	MOTA	529	0	HIS.	Α :	100	61.700	77.745	19.959	1.00	62.72
	ATOM	530	CB	HIS .	A :	100	59.934	79.519	21.936	1.00	65.08
55	ATOM	531	CG	HIS .			59.490	80.812	22.561		65.42
	MOTA	532		HIS			58.685	81.717	21.904		65.80
	MOTA	533		HIS A			59.702	81.330	23.797		66.64
	ATOM	534	CEl	HIS A	A.	100	58.441	82.748	22.696		66.12
	MOTA	535	NE2	HIS .	Α.	100	59.045	82.536	23.852	1.00	65.68
60	ATOM	536	N	SER .			62.175	77.146	22.071		63.26
-	ATOM	537	CA	SER A			62.407	75.760	21.703		62.93
		538									
	ATOM		C	SER A			61.049	75.092	21.406		62.18
	ATOM	539	0	SER A			60.140	75.073	22.242		61.25
	MOTA	540	CB	SER A	A :	101	63.161	75.034	22.823		63.06
65	MOTA	541	OG	SER A			63.767	73.844	22.335		63.28
	ATOM	542	N	ILE A			60.910	74.552	20.204		61.55
	ATOM	543	CA								
				ILE A			59.650	73.964	19.801		60.98
	ATOM	544	C	ILE A			59.558	72.519	20.239		59.90
	MOTA	545	0	ILE A			60.478	71.751	20.018	1.00	60.20
70	MOTA	546	CB	ILE A	Α :	102	59.487	74.108	18.302		61.31

5	ATOM ATOM	547 548 549 550 551 552 553	CG: CD: N CA C	2 ILE A 1 ILE A ASN A ASN A ASN A	102 102 103 103 103 103	59.204 58.343 59.190 58.446 58.283 57.658 58.051	73.215 75.918 72.154 70.808 69.826 68.671	17.988 17.805 16.529 20.873 21.419 20.430 20.332	1.00 61.95 1.00 61.93 1.00 58.45 1.00 57.23 1.00 56.00
10	ATOM ATOM ATOM ATOM ATOM	554 555 556 557 558	CG OD1 ND2 N	ASP A	103 103 103 104	57.440 57.481 56.598 58.507 56.663	69.554 68.714 69.389 70.277	22.706 23.496 23.352 24.348 19.702	1.00 57.35 1.00 57.35 1.00 55.48 1.00 56.22 1.00 55.10
15	ATOM ATOM ATOM ATOM ATOM ATOM	559 560 561 562 563 564	CA C O CB CG	ASP A ASP A ASP A ASP A	104 104 104 104	56.014 55.324 55.329 55.018 54.749	69.397 70.283 71.511 68.470 67.177	18.765 17.769 17.921 19.477 18.699	1.00 54.05 1.00 55.23 1.00 56.71
20	ATOM ATOM ATOM ATOM ATOM	565 566 567 568 569	OD2 N CA C	ASP A TYR A TYR A TYR A TYR A TYR A	104 105 105 105	55.381 53.919 54.736 54.086 52.838 52.726	66.957 66.320 69.656 70.356 69.609 68.403	17.647 19.064 16.764 15.687 15.319 15.543	1.00 55.96 1.00 60.44 1.00 52.66 1.00 52.56 1.00 51.25
25	ATOM ATOM ATOM ATOM ATOM	570 571 572 573 574	CB CG	TYR A TYR A TYR A TYR A	105 105 105 105	54.976 55.070 54.132 56.087 54.204	70.362 69.000 68.603 68.106 67.347	13.543 14.448 13.774 12.829 14.096 12.215	1.00 51.29 1.00 53.10 1.00 55.91 1.00 59.33 1.00 58.18
30	ATOM ATOM ATOM ATOM ATOM	575 576 577 578 579	CE2 CZ OH N		105 105 105 106	56.169 55.231 55.300 51.899 50.719	66.855 66.485 65.245 70.313 69.644	12.215 13.483 12.542 11.937 14.724 14.246	1.00 60.78 1.00 59.77 1.00 60.60 1.00 60.13 1.00 49.68
35	ATOM ATOM ATOM ATOM ATOM	580 581 582 583 584	C O CB OG N	SER A SER A SER A SER A ILE A	106 106 106 106	50.252 49.835 49.614 48.498	70.331 71.499 69.625 68.968	12.986 12.976 15.291 14.757	1.00 49.10 1.00 48.51 1.00 47.69 1.00 48.76 1.00 48.08
40	ATOM ATOM ATOM ATOM ATOM	585 586 587 588 589	CA C O CB	ILE A ILE A ILE A	107 107 107 107	50.272 49.959 48.473 47.875 50.820	69.567 70.124 70.005 68.975 69.433	11.920 10.650 10.454 10.737 9.595	1.00 47.91 1.00 48.19 1.00 48.08 1.00 47.65 1.00 48.45
45	ATOM ATOM ATOM ATOM	590 591 592 593	CG2 CD1 N CA	ILE A ILE A ILE A SER A SER A	107 107 108 108	52.193 50.856 53.411 47.860 46.445	69.181 70.256 69.417 71.104 71.086	10.252 8.325 9.444 10.053 9.814	1.00 48.77 1.00 48.58 1.00 50.54 1.00 48.44 1.00 49.14
50	ATOM ATOM ATOM ATOM	594 595 596 597 598	C O CB OG N	SER A SER A SER A PRO A	108 108 108 109	46.247 47.165 45.958 46.787 45.062	70.064 69.818 72.469 73.035 69.465	7.946 9.394 8.386 8.631	1.00 50.02 1.00 49.19 1.00 50.05 1.00 50.74
55	ATOM ATOM ATOM ATOM ATOM	599 600 601 602 603	CA C O CB CG	PRO A PRO A PRO A PRO A	109 109 109 109	44.782 44.722 44.922 43.390 43.059	68.440 68.956 68.161 67.936 68.544	7.617 6.185 5.264 7.981 9.324	1.00 50.80 1.00 51.14 1.00 51.45 1.00 50.92 1.00 51.33
60	ATOM ATOM ATOM ATOM ATOM	604 605 606 607 608	CD N CA C	PRO A ASP A ASP A ASP A	110 110 110	43.907 44.391 44.352 45.715 45.851	69.734 70.219 70.690 71.225 71.807	9.501 5.965 4.590 4.196 3.139	1.00 50.54 1.00 50.90 1.00 51.01 1.00 51.06 1.00 52.40
65	ATOM ATOM ATOM ATOM ATOM	609 610 611 612 613		ASP A ASP A ASP A GLY A	110 110 110	43.227 43.344 44.363 42.466 46.725	71.703 72.955 73.103 73.853 71.007	4.328 5.182 5.860 5.223 5.031	1.00 50.49 1.00 49.53 1.00 45.06 1.00 49.22 1.00 51.13
70	MOTA MOTA MOTA	614 615 616	CA C O	GLY A GLY A GLY A	111 111	48.084 48.338 49.409	71.465 72.982 73.417	4.746 4.684 4.250	1.00 51.15 1.00 51.16 1.00 51.30 1.00 51.86

	MOTA MOTA MOTA	617 618 619	N CA C	GLN A GLN A GLN A	112 112	47.386 47.535 48.236	73.797 75.249 75.898	5.127 5.078 6.299	1.00 1.00	50.80 50.53 49.99
5	ATOM ATOM ATOM ATOM	620 621 622 623	O CB CG CD	GLN A GLN A GLN A GLN A	112 112	48.706 46.149 45.484 44.189	77.038 75.872 75.478 76.236	6.238 4.878 3.555 3.297	1.00 1.00	49.93 50.71 51.08 52.53
10	ATOM ATOM	624 625 626	OE1 NE2		112	44.104 43.179 48.318	77.442 75.533 75.191	3.556 2.798 7.414	1.00	53.75 51.77 49.50
10	ATOM ATOM	627 628	N CA C	PHE A PHE A	113 113	48.899 49.547	75.781 74.749	8.613 9.488	1.00	48.63 48.52
15	ATOM ATOM ATOM	629 630 631	O CB CG	PHE A PHE A PHE A	113	49.183 47.818 46.954	73.567 76.424 77.415	9.479 9.488 8.782	1.00	48.60 48.00 47.61
	ATOM ATOM	632 633	CD1 CD2	PHE A PHE A	113 113	47.307 45.777	78.752 77.025	8.741 8.185	1.00	47.99 46.46
20	ATOM ATOM ATOM	634 635 636	CE1 CE2	PHE A PHE A PHE A	113	46.503 44.969 45.333	79.673 77.950 79.271	8.092 7.540 7.491	1.00	47.46 47.60 47.63
	ATOM ATOM ATOM	637 638 639	N CA C	ILE A ILE A ILE A	114	50.470 51.071 50.970	75.220 74.359 74.974	10.309 11.288 12.683	1.00	48.29 48.07 47.45
25	ATOM ATOM	640 641	O CB	ILE A ILE A	114 114	51.136 52.529	76.180 74.065	12.853 10.915	1.00	46.70 48.57 48.34
	ATOM ATOM ATOM	642 643 644	CG1 CG2 CD1	ILE A ILE A ILE A	114 114	53.144 53.324 54.622	73.118 75.366 72.906	11.949 10.775 11.770	1.00	48.17 50.52
30	ATOM ATOM ATOM	645 646 647	N CA C	LEU A LEU A LEU A	115	50.670 50.656 52.013	74.118 74.482 74.192	13.660 15.064 15.606	1.00	46.94 46.46 45.85
	ATOM ATOM ATOM	648 649 650	O CB CG	LEU A LEU A LEU A	115	52.494 49.717 48.381	73.087 73.572 74.042	15.461 15.849 16.381	1.00	45.54 46.47 48.15
35	ATOM ATOM	651 652	CD1 CD2	LEU A LEU A	115 115	47.816 48.504	72.910 75.302	17.237 17.189	1.00	48.28 48.34
	ATOM ATOM ATOM	653 654 655	N CA C	LEU A LEU A	116	52.608 53.872 53.597	75.154 74.950 74.957	16.282 16.952 18.447	1.00	45.86 45.94 45.74
40	ATOM ATOM ATOM	656 657 658	O CB CG	LEU A LEU A LEU A	116 116	53.005 54.849 55.204	75.875 76.077 76.301	18.958 16.616 15.150	1.00 1.00	45.58 46.09 46.93
45	ATOM ATOM ATOM	659 660 661	CD1 CD2 N	LEU A LEU A GLU A	116	56.002 55.989 54.048	77.596 75.160 73.936	15.013 14.614 19.156	1.00	48.50 48.06 46.50
13	ATOM ATOM	662 663	CA C	GLU A GLU A	117 117	53.799 55.084 56.114	73.818 74.081 73.520	20.587 21.341 21.027	1.00	46.10 45.85 46.64
50	ATOM ATOM ATOM	664 665 666	O CB CG	GLU A GLU A	117 117	53.295 53.051	72.405 72.060	20.871 22.332	1.00	46.38 46.56
	ATOM ATOM ATOM	667 668 669	CD OE1 OE2	GLU A GLU A	117	52.655 51.560 53.434	70.594 70.188 69.852	22.516 22.081 23.130	1.00	46.13 44.34 48.23
55	ATOM ATOM ATOM	670 671 672	N CA C	TYR A TYR A TYR A	118	55.045 56.261 55.894	74.930 75.224 75.555	22.347 23.081 24.530	1.00	45.50 44.57 44.74
	ATOM ATOM ATOM	673 674 675	O CB CG	TYR A TYR A TYR A	118	54.712 57.021 56.363	75.640 76.347 77.714	24.860 22.360 22.363	1.00	44.74 44.78 43.33
60	ATOM ATOM ATOM	676 677 678	CD1 CD2 CE1	TYR A TYR A TYR A	118 118	55.410 56.732 54.826	78.056 78.666 79.311	21.429 23.276 21.428	1.00	43.21 42.55 42.60
. -	ATOM ATOM	679 680	CE2	TYR A	118 118	56.149 55.200	79.908 80.222	23.289 22.362	1.00 1.00	42.33 42.64
65	ATOM ATOM	681 682 683	OH N CA	TYR A ASN A ASN A	119 119	54.635 56.883 56.610	81.462 75.719 75.968	22.379 25.399 26.805	1.00 1.00	43.87 44.34 44.35
70	ATOM ATOM ATOM	684 685 686	C O CB	ASN A ASN A	119	55.799 54.819 55.826	74.775 74.960 77.282	27.389 28.116 27.002	1.00	43.75 42.59 44.61

	ATOM ATOM ATOM	687 688 689		ASN		57.	673 911	78.550 78.515	26.780 26.675	1.00 46.44 1.00 48.82
5	ATOM	690 691 692 693	N CA C C	TYR .	A 120 A 120 A 120 A 120 A 120	56. 55. 55.	536 849	79.688 73.564 72.357 72.045	26.725 27.031 27.460 28.917	1.00 46.66 1.00 42.78 1.00 42.17 1.00 41.40
10	ATOM ATOM ATOM ATOM	694 695 696 697	CB CG CD1 CD2	TYR . TYR .	A 120 A 120 A 120 A 120 A 120	57. 55. 55. 56. 54.	932 770 670	71.900 71.195 69.805 69.324 68.982	29.320 26.543 27.131 28.058 26.757	1.00 40.43 1.00 43.02 1.00 43.77 1.00 45.93
15	ATOM ATOM ATOM ATOM	698 699 700 701	CE1 CE2 CZ OH	TYR A	A 120 A 120 A 120 A 120 A 120	56. 54. 55.	542 573 489	68.063 67.712 67.265 66.029	28.592 27.295 28.204 28.766	1.00 44.47 1.00 46.89 1.00 44.14 1.00 45.39 1.00 45.22
	ATOM ATOM ATOM ATOM	702 703 704 705	N CA C O		A 121 A 121 A 121	54.1 54.1 54.1	806 974 123	71.982 71.605 70.370 70.408	29.725 31.121 31.318 31.166	
20	ATOM ATOM ATOM ATOM	706 707 708 709	CB CG1 CG2 N	VAL A	A 121 A 121 A 121	54.5 54.5 55.3	554 784 362	72.713 72.295 73.994 69.270	32.051 33.502 31.720 31.616	1.00 39.90 1.00 40.45 1.00 41.03 1.00 35.67
25	MOTA MOTA ATOM MOTA	710 711 712 713	CA C O CB	LYS A LYS A LYS A	122 122	54.0 53.2 53.6 55.0	217 673	68.033 68.015 68.378 66.876	31.821 33.063 34.146 31.952	1.00 35.20 1.00 34.14 1.00 33.72 1.00 35.21
30	ATOM ATOM ATOM ATOM ATOM	714 715 716 717 718	CG CD CE NZ N	LYS A LYS A LYS A GLN A	122 122 122	54.3 55.2 54.4 54.9	212 169 953	65.582 64.328 63.297 61.959	32.319 32.387 33.288 33.075	1.00 36.44 1.00 38.33 1.00 40.56 1.00 41.12
35	ATOM ATOM ATOM ATOM	719 720 721 722	CA C O CB	GLN A GLN A GLN A GLN A	123 123 123	51.9 51.1 51.1 52.0 49.7	L37 L41)73	67.512 67.272 65.798 65.318 67.800	32.913 34.086 34.419 34.997 33.922	1.00 32.33 1.00 31.49 1.00 29.73 1.00 29.32 1.00 31.37
40	ATOM ATOM ATOM ATOM ATOM	723 724 725 726 727	CG CD OE1 NE2	GLN A GLN A GLN A	123 123 123 123	49.0 47.5 47.1 46.8	014 565 118 810	67.763 68.168 68.685 67.879	35.303 35.344 36.364 34.295	1.00 32.48 1.00 35.18 1.00 41.34 1.00 33.83
45	ATOM ATOM ATOM ATOM	727 728 729 730 731	N CA C O CB	TRP A TRP A TRP A TRP A	124 124 124	50.1 50.1 50.6 51.4 48.7	.26 49 196	65.046 63.619 62.794 63.257 63.166	34.049 34.389 33.216 32.505 34.862	1.00 29.19 1.00 28.77 1.00 28.48 1.00 29.03 1.00 28.15
	ATOM ATOM ATOM ATOM	732 733 734 735	CG CD1 CD2	TRP A TRP A TRP A TRP A	124 124 124	48.1 46.9 48.7 46.7	.71 6 .71 6 .67 6	64.047 64.654 64.407 65.373	35.916 35.882	1.00 28.17 1.00 28.36 1.00 28.10 1.00 26.42
50	ATOM ATOM ATOM ATOM	736 737 738 739	CE2 CE3 CZ2	TRP A TRP A TRP A	124 124 124	47.8 49.9 48.1 50.2	46 6 88 6 02 6	55.242 54.099 55.801 54.652	37.841 37.798 39.107 39.056	1.00 27.48 1.00 24.94 1.00 24.59 1.00 26.05
55	ATOM ATOM ATOM ATOM	740 741 742 743	CH2 N CA	TRP A ARG A ARG A ARG A	124 125 125	49.2 50.1 50.6 50.3	86 6 64 6 57 6	55.477 51.579 50.764 51.345	39.709 33.003 31.907 30.519	1.00 24.28 1.00 29.19 1.00 29.06 1.00 29.40
60	ATOM ATOM ATOM ATOM	744 745 746 747	CB CG CD	ARG A ARG A ARG A ARG A	125 125 125	51.2 50.1 50.7 50.1	12 6 03 5 96 5	51.246 59.330 58.308 56.928	29.642 31.998 31.001 30.934	1.00 28.73 1.00 29.53 1.00 29.97 1.00 27.63
65	ATOM ATOM ATOM ATOM	748 749 750 751	CZ NH1 NH2	ARG A ARG A ARG A	125 125 125	50.04 50.93 52.13 50.74	45 5 84 5 24 5 80 5	66.297 55.535 55.282 55.005	32.248 32.814 32.191 34.015	1.00 28.44 1.00 30.55 1.00 29.95 1.00 29.23
	ATOM ATOM ATOM ATOM	752 753 754 755	CA C	HIS A HIS A HIS A HIS A	126 126	49.23 48.93 48.74 49.03	22 6 46 6	1.961 2.516 4.039 4.700	30.300 28.977 28.988 27.993	1.00 29.58 1.00 29.53 1.00 29.76 1.00 30.56
70	MOTA	756	CB :	HIS A	126	47.65		1.858	28.416	1.00 29.39

	ATOM ATOM ATOM	757 758 759	CG ND1 CD2		6 48.42	9 59.602	27.596	1.00 29.10 1.00 24.61 1.00 31.06
5	ATOM ATOM ATOM ATOM	760 761 762 763	CE1 NE2 N CA	HIS A 12	6 48.26 6 47.48 7 48.26	2 58.321 9 58.216 2 64.586	27.869 28.941	1.00 27.22 1.00 27.52 1.00 28.69 1.00 27.65
10	ATOM ATOM ATOM ATOM	764 765 766 767	C O CB OG	SER A 12 SER A 12 SER A 12 SER A 12	7 49.33 7 50.38 7 47.19	8 66.828 1 66.369 0 66.282	30.359 30.886 31.491 32.617	1.00 28.78 1.00 27.69 1.00 28.00 1.00 23.91
15	ATOM ATOM ATOM ATOM	768 769 770 771	N CA C	TYR A 12 TYR A 12 TYR A 12 TYR A 12	8 49.24 8 50.32 8 49.77	4 68.059 8 69.009 6 70.328	29.890 29.997 29.587 29.051	1.00 29.78 1.00 31.21 1.00 31.31 1.00 30.93
	ATOM ATOM ATOM ATOM	772 773 774 775	CB CG CD1 CD2	TYR A 123 TYR A 123 TYR A 123 TYR A 123	3 51.47 3 51.10 51.00	6 68.615 8 68.469 9 69.582	29.063 27.608 26.785 27.036	1.00 31.91 1.00 32.71 1.00 36.05 1.00 35.28
20	ATOM ATOM ATOM ATOM	776 777 778 779	CE1 CE2 CZ OH	TYR A 123 TYR A 123 TYR A 123	3 50.57 3 50.50	2 69.452 0 67.073 7 68.190	25.436 25.686 24.897 23.563	1.00 34.89 1.00 33.91 1.00 34.61 1.00 35.38
25	ATOM ATOM ATOM ATOM	780 781 782 783	N CA C O	THR A 129 THR A 129 THR A 129 THR A 129	50.09 51.20	72.681 73.142	29.901 29.340 28.423 28.518	1.00 32.61 1.00 33.63 1.00 33.39 1.00 32.91
30	ATOM ATOM ATOM ATOM	784 785 786 787	CB OG1 CG2 N	THR A 129 THR A 129 THR A 129 ALA A 130	50.974 48.60	73.693 73.488	30.395 31.337 31.192 27.580	1.00 34.35 1.00 35.37 1.00 35.67 1.00 33.49
35	ATOM ATOM ATOM ATOM	788 789 790 791	CA C O CB	ALA A 130 ALA A 130 ALA A 130 ALA A 130	51.220 50.034	75.987 76.359	26.616 25.993 26.172 25.512	1.00 34.05 1.00 34.58 1.00 34.01 1.00 33.60
	ATOM ATOM ATOM ATOM	792 793 794 795	N CA C O	SER A 131 SER A 131 SER A 131	52.139 51.879 51.829	76.655 77.851 77.419	25.266 24.480 23.032 22.657	1.00 34.97 1.00 35.90 1.00 37.17 1.00 36.47
40	ATOM ATOM ATOM ATOM	796 797 798 799	CB OG N CA	SER A 131 SER A 131 TYR A 132 TYR A 132	53.034 53.004 51.084	78.835 79.607 78.135	24.570 25.730 22.205 20.820	1.00 36.15 1.00 35.91 1.00 38.73 1.00 41.07
45	ATOM ATOM ATOM ATOM	800 801 802 803	C O CB CG	TYR A 132 TYR A 132 TYR A 132 TYR A 132	51.063 50.642 49.605	78.887 80.002 77.030	19.845 20.108 20.581 21.185	1.00 42.38 1.00 42.56 1.00 41.24
50	ATOM ATOM ATOM ATOM	804 805 806 807	CD1 CD2 CE1 CE2	TYR A 132 TYR A 132 TYR A 132 TYR A 132	50.010 49.131 50.006 49.128	74.563 75.478 73.296 74.240	20.487 22.486 21.071 23.073	1.00 42.55 1.00 44.60 1.00 44.31
55	ATOM ATOM ATOM ATOM ATOM	808 809 810 811 812	CZ OH N CA C	TYR A 132 TYR A 133 ASP A 133 ASP A 133	49.550 51.625 51.641	71.915 78.584 79.536	22.362 22.958 18.699 17.614 16.398	1.00 43.70 1.00 44.24 1.00 44.24 1.00 46.11 1.00 46.98
60	ATOM ATOM ATOM ATOM	813 814 815 816	O CB CG	ASP A 133 ASP A 133 ASP A 133 ASP A 133	51.206 53.055 53.341	77.598 80.053 81.301	16.306 17.361 18.110	1.00 47.50 1.00 46.19 1.00 46.73
00	ATOM ATOM ATOM	817 818 819	OD2 N CA	ASP A 133 ILE A 134 ILE A 134	54.490 50.547 50.161	81.754 79.573 78.994	18.640 18.227 15.484 14.243	1.00 47.58 1.00 51.67 1.00 48.21 1.00 49.72
65	ATOM ATOM ATOM ATOM	820 821 822 823	C O CB CG1	ILE A 134 ILE A 134 ILE A 134	50.922 48.702 47.917	80.919 79.124 78.658	13.159 13.063 13.999 15.216	1.00 51.48 1.00 51.56 1.00 49.74 1.00 50.32
70	ATOM ATOM ATOM	82 4 825 826		ILE A 134 ILE A 134 TYR A 135	46.477	79.187	12.797 15.260 12.356	1.00 49.73 1.00 50.42 1.00 53.32
70	MOTA	825	CD1	ILE A 134	46.477	79.187	15.260	1.00 50.42

	ATOM	82	7 C#	YYR	A 135	52.464	79.424	11.279	1 00	54.70
	ATOM	82			A 135	51.735				55.69
	MOTA	82			A 135	51.351				55.37
	ATOM	83	-		A 135	53.840			1.00	
5	ATOM	83:			A 135	54.844			1.00	
	ATOM	832			A 135	55.449			1.00	
	ATOM	833	CE		A 135	55.203				58.33
	ATOM	834			A 135	56.381				59.70
	MOTA	835			A 135	56.123				60.29
10	ATOM	836			A 135	56.714				60.03
	MOTA	837			A 135	57.632	80.157			61.36
	ATOM	838	3 N		A 136	51.508	80.166			57.00
	ATOM	839	CA		A 136	50.751	80.082		1.00	
	ATOM	840) C		A 136	51.661	79.653	6.795		59.15
15	ATOM	841	. 0	ASP	A 136	52.551	80.379	6.416	1.00	
	ATOM	842	CB		A 136	50.148	81.448	7.586	1.00	
	ATOM	843	CG	ASP	A 136	49.311	81.463	6.304	1.00	58.07
	MOTA	844		1 ASP		49.647	80.776	5.305	1 00	56.04
	MOTA	845	OD	2 ASP	A 136	48.292	82.190	6.228		58.58
20	MOTA	846			A 137	51.386	78.489	6.233		61.13
	ATOM	847	CA	LEU	A 137	52.306	77.855	5.295		62.59
	ATOM	848	_	LEU	A 137	52.425	78.444	3.901	1.00	63.90
	ATOM	849			A 137	53.532	78.530	3.382	1.00	63.88
	MOTA	850			A 137	51.990	76.368	5.198	1.00	62.65
25	ATOM	851			A 137	52.645	75.596	6.341	1.00	
	ATOM	852		1 LEU		51.922	74.310	6.631	1.00	63.27
	ATOM	853		2 LEU		54.088	75.327	5.981	1.00	63.98
	ATOM	854	N		A 138	51.315	78.829	3.284		65.63
20.	ATOM	855	CA		A 138	51.375	79.327	1.907	1.00	66.97
30	ATOM	856	C		A 138	52.144	80.633	1.857		67.75
	ATOM	857	0		A 138	52.926	80.893	0.935		68.07 [.]
	ATOM ATOM	858	CB		A 138	49.975	79.431	1.304		67.06
	ATOM	859 860	CG		A 138	49.442	78.077	0.889		67.65
35	ATOM	861		l asn 2 2 asn 2		50.227	77.151	0.629		68.25
55	ATOM	862	N		A 136	48.108	77.938	0.842		67.87
	ATOM	863	CA		A 139	51.910	81.448	2.873		68.62
	ATOM	864	C		A 139	52.738 53.816	82.607	3.119		69.62
	ATOM	865	ŏ	LYS A		53.810	81.972 80.750	3.992		69.94
40	ATOM	866	ČВ	LYS A		51.935	83.672	4.037		70.33
	ATOM	867	CG	LYS A		50.611	83.997	3.855 3.158		69.82
	ATOM	868	CD	LYS A		49.587	84.614	4.104		70.97 73.07
	ATOM	869	CE	LYS A		48.174	84.576	3.502	1.00	
	ATOM	870	NZ	LYS A		47.102	84.617	4.550	1.00	
45	MOTA	871	N	ARG A	140	54.655	82.754	4.660	1.00	
	ATOM	872	CA	ARG A		55.630	82.191	5.602		70.26
	ATOM	873	С	ARG A	140	55.494	82.987	6.880	1.00	
	ATOM	874	0	ARG A	140	56.477	83.343	7.526		
	ATOM	875	CB	ARG A		57.044	82.353	5.077	1.00	
50	ATOM	876	CG	ARG A		57.257	81.894	3.659	1.00	
	ATOM	877	CD	ARG A		58.665	82.214	3.142	1.00	76.89
	ATOM	878	NE	ARG A		58.778	82.051	1.694	1.00	79.70
	ATOM	879	CZ	ARG A		58.291	82.904	0.792	1.00	82.20
55	ATOM	880	NHI	ARG A	140	57.656	84.008	1.168	1.00	82.19
23	ATOM	881		ARG A		58.458	82.654	-0.500	1.00	83.24
	ATOM	882	N	GLN A		54.250	83.240	7.249	1.00	
	ATOM	883	CA	GLN A		53.934	84.207	8.282	1.00	
	ATOM ATOM	884	C	GLN A		53.402	83.537	9.525	1.00	
60		885	0	GLN A		52.499	82.716	9.457	1.00	
00	ATOM	886	CB	GLN A		52.851	85.142	7.718	1.00	68.09
	ATOM ATOM	887	CG	GLN A		52.822	86.583	8.222	1.00	
	ATOM	888 889	CD OF1	GLN A		51.681	87.394	7.570		71.88
	ATOM	890		GLN A		50.694	87.749	8.226		72.03
65	ATOM	891				51.811	87.654	6.273		72.19
55	ATOM	892	N CA	LEU A		53.984	83.871	10.659	1.00	
	ATOM	893	CA	LEU A		53.403	83.477	11.916	1.00	
	ATOM	894	0	LEU A		52.126	84.298	12.008	1.00	
	ATOM	895	СВ	LEU A		52.021 54.330	85.355	11.388	1.00	
70	ATOM	896	CG	LEU A		55.543	83.840	13.067	1.00 6	
-				TLU A	1 7 C	22.243	82.928	13.195	1.00 6	5.68

	ATOM	897		LEU A 14		56.665	83.608	13.991	1.00 66.52
	ATOM ATOM	898 899	CD2 N	LEU A 14 ILE A 14		55.130 51.143	81.600 83.830	13.821 12.757	1.00 65.75 1.00 62.15
	ATOM	900	CA	ILE A 14	3	49.930	84.618	12.900	1.00 61.48
5	ATOM	901	C	ILE A 14 ILE A 14		50.038 50.387	85.417 84.867	14.190 15.221	1.00 60.32 1.00 60.32
	ATOM ATOM	902 903	O CB	ILE A 14		48.690	83.724	12.870	1.00 61.54
	ATOM	904	CG1			48.543	83.144	11.468	1.00 61.17
10	ATOM ATOM	905 906	CG2 CD1	ILE A 14 ILE A 14		47.454 47.407	84.528 82.228	13.238 11.299	1.00 61.79 1.00 61.35
10	ATOM	907	N	THR A 14	4	49.773	86.716	14.115	1.00 58.81
	ATOM	908 909	CA	THR A 14 THR A 14		49.916 48.555	87.586 87.935	15.263 15.856	1.00 58.06 1.00 57.10
	ATOM ATOM	919	C O	THR A 14		48.469	88.455	16.963	1.00 57.10
15	ATOM	911	CB	THR A 14		50.670	88.874	14.869	1.00 58.11
	ATOM ATOM	912 913	OG1 CG2	THR A 14 THR A 14		51.839 51.246	88.550 89.585	14.118 16.105	1.00 58.85 1.00 59.32
	ATOM	914	N	GLU A 14	5	47.501	87.614	15.126	1.00 55.99
20	ATOM	915 916	CA	GLU A 14 GLU A 14		46.136 45.459	87.937 86.793	15.513 16.258	1.00 55.66 1.00 54.33
20	ATOM ATOM	917	C O	GLU A 14		45.570	85.638	15.850	1.00 53.39
	ATOM	918	CB	GLU A 14		45.332	88.143	14.237	1.00 56.14
	ATOM ATOM	919 920	CG CD	GLU A 14 GLU A 14		44.515 44.375	89.407 89.792	14.110 12.642	1.00 58.11 1.00 60.69
25	ATOM	921	OE1	GLU A 14	5	45.384	90.216	12.048	1.00 62.49
	ATOM	922	OE2	GLU A 14		43.283 44.733	89.628 87.134	12.059 17.321	1.00 62.39 1.00 53.21
	ATOM ATOM	923 924	N CA	GLU A 14 GLU A 14		43.890	86.192	18.050	1.00 52.46
••	ATOM	925	C	GLU A 14	5	44.601	84.893	18.376	1.00 51.84
30	ATOM ATOM	926 927	O CB	GLU A 14 GLU A 14		44.125 42.654	83.806 85.904	18.042 17.206	1.00 51.80 1.00 52.69
	ATOM	928	CG	GLU A 14		41.898	87.159	16.814	1.00 52.58
	MOTA	929 930	CD OE1	GLU A 14		41.272 41.243	87.854 87.256	18.007 19.090	1.00 52.40 1.00 51.55
35	ATOM ATOM	931	OE2	GLU A 14		40.809	88.995	17.868	1.00 53.65
	ATOM	932	N	ARG A 14		45.749	85.011	19.021	1.00 50.64
	ATOM ATOM	933 934	CA C	ARG A 14'		46.569 45.949	83.861 82.956	19.314 20.325	1.00 50.07 1.00 48.87
	ATOM	935	0	ARG A 14	7	45.159	83.385	21.170	1.00 48.31
40	ATOM ATOM	936 937	CB CG	ARG A 14		47.891 48.732	84.314 85.057	19.880 18.901	1.00 50.41 1.00 53.00
	ATOM	938	CD	ARG A 14		50.090	85.381	19.439	1.00 55.81
	ATOM	939 940	NE	ARG A 14		50.998 52.324	85.691 85.592	18.348 18.415	1.00 60.02 1.00 64.02
45	ATOM ATOM	941	CZ NH1	ARG A 14		52.914	85.181	19.536	1.00 63.93
	ATOM	942	NH2	ARG A 14		53.065	85.902	17.350	1.00 66.19 1.00 47.51
	ATOM ATOM	943 944	N CA	ILE A 14:		46.333 45.945	81.691 80.711	20.238 21.217	
	ATOM	945	C	ILE A 14	3	46.600	81.226	22.488	1.00 45.49
50	ATOM ATOM	946 947	O CB	ILE A 14:		47.712 46.454	81.697 79.320	22.446 20.816	1.00 45.33 1.00 46.49
	ATOM	948	CG1	ILE A 14		45.726	78.846	19.554	1.00 46.40
	ATOM	949	CG2	ILE A 14		46.192	78.311	21.917	1.00 46.14 1.00 47.77
55	ATOM ATOM	950 951	CD1 N	ILE A 14		46.344 45.906	77.600 81.209	18.955 23.605	1.00 47.77
	ATOM	952	CA	PRO A 14	9	46.501	81.726	24.840	1.00 43.90
	ATOM ATOM	953 954	С О	PRO A 14		47.525 47.553	80.798 79.610	25.484 25.221	1.00 42.87 1.00 41.74
	ATOM	955	СВ	PRO A 14		45.324	81.848	25.799	1.00 43.71
60	ATOM	956	CG	PRO A 14		44.149	81.190	25.135 23.783	1.00 45.01 1.00 44.57
	ATOM ATOM	957 958	CD N	PRO A 14:		44.537 48.336	80.710 81.387	26.353	1.00 42.54
	ATOM	959	CA	ASN A 15)	49.270	80.668	27.189	1.00 42.35
65	ATOM ATOM	960 961	С 0	ASN A 15		48.520 47.369	79.769 80.033	28.137 28.475	1.00 40.60 1.00 40.98
03	ATOM	962	СВ	ASN A 15)	50.128	81.645	28.009	1.00 43.01
	ATOM	963	CG OD1	ASN A 15		51.107 51.764	82.422 81.853	27.153 26.283	1.00 45.14 1.00 44.71
	ATOM ATOM	964 965		ASN A 15		51.764	83.745	26.283	1.00 44.71
70	ATOM	966	N	ASN A 15		49.197	78.715	28.579	1.00 39.29

ATOM 971 CG ASN A 151 49.484 79.088 31.515 1.00 40.57 ATOM 973 ND2 ASN A 151 49.486 80.411 31.508 1.00 47.51 ATOM 974 N THR A 152 46.381 76.084 26.917 1.00 35.12 ATOM 975 CA THR A 152 46.381 76.084 26.917 1.00 35.12 ATOM 976 C THR A 152 46.579 74.644 27.930 1.00 35.12 ATOM 977 O THR A 152 47.716 74.159 27.346 1.00 32.32 ATOM 978 CB THR A 152 47.716 74.159 27.346 1.00 32.32 ATOM 979 OGI THR A 152 45.978 77.550 25.079 1.00 34.54 ATOM 980 CG2 THR A 152 45.978 77.550 25.079 1.00 34.54 ATOM 981 N GLN A 153 45.461 73.960 27.524 1.00 32.13 ATOM 982 C GLN A 153 45.485 72.602 28.045 1.00 32.33 ATOM 983 C GLN A 153 45.485 72.602 28.045 1.00 32.33 ATOM 984 C GLN A 153 45.831 71.526 26.970 1.00 33.22 20 ATOM 986 C GLN A 153 45.831 71.526 26.970 1.00 33.22 ATOM 987 CD GLN A 153 45.801 72.446 29.144 1.00 31.28 ATOM 988 C GLN A 153 44.401 72.446 29.144 1.00 31.28 ATOM 988 OEI GLN A 153 44.401 72.446 29.144 1.00 31.28 ATOM 988 OEI GLN A 153 44.401 72.446 29.144 1.00 31.28 ATOM 988 OEI GLN A 153 44.401 72.446 29.145 1.00 32.66 ATOM 999 N TRP A 154 44.658 71.838 25.883 1.00 22.53 ATOM 999 N TRP A 154 44.658 71.838 25.883 1.00 22.53 ATOM 999 N TRP A 154 44.658 71.838 25.883 1.00 32.73 ATOM 999 OT TRP A 154 44.155 70.907 24.769 1.00 33.22 ATOM 999 OT TRP A 154 44.155 70.907 24.769 1.00 33.23 ATOM 999 OT TRP A 154 44.155 70.907 24.769 1.00 33.23 ATOM 999 OT TRP A 154 44.155 70.907 24.769 1.00 33.23 ATOM 999 OT TRP A 154 44.155 70.907 24.769 1.00 33.23 ATOM 999 OT TRP A 154 44.155 70.907 24.769 1.00 33.23 ATOM 999 OT TRP A 154 44.155 70.907 24.769 1.00 33.23 ATOM 999 OT TRP A 154 44.155 70.907 24.769 1.00 33.23 ATOM 999 OT TRP A 154 44.155 70.907 24.769 1.00 33.23 ATOM 999 OT TRP A 154 44.155 70.907 24.769 1.00 33.23 ATOM 999 OT TRP A 154 44.155 70.907 25.88 1.00 30.752 ATOM 990 OT TRP A 154 44.155 70.907 25.88 1.00 30.752 ATOM 990 OT TRP A 154 44.155 70.907 25.88 1.00 30.353 ATOM 990 OT TRP A 155 44.1007 25.88 1.00 30.3559 ATOM 990 OT TRP A 156 42.209 70.907 24.769 1.00 33.33 30 ATOM 990 OT TRP A 156 42.209 70.907 24.769 1.00 33.33		ATOM ATOM ATOM ATOM	967 968 969 970	C	ASN ASN	A 151 A 151 A 151 A 151	48.637 47.429 46.544 48.284	77.004 76.538		1.00 36.63 1.00 34.40
ATOM 975 CA THIR A 152 46.381 76.084 26.917 1.00 34.25 ATOM 976 C THIR A 152 47.716 74.159 27.346 1.00 33.21 ATOM 978 CB THIR A 152 47.716 74.159 27.346 1.00 33.21 ATOM 979 OG1 THIR A 152 47.716 74.159 27.346 1.00 34.54 ATOM 980 CG2 THIR A 152 45.978 77.550 25.079 1.00 34.54 ATOM 980 CG2 THIR A 152 45.978 77.550 25.079 1.00 34.54 ATOM 981 N GEN A 153 45.440 73.960 27.524 1.00 34.54 ATOM 982 CG GEN A 153 45.485 72.602 28.045 1.00 32.33 ATOM 983 C GEN A 153 45.485 72.602 28.045 1.00 32.33 ATOM 985 CB GEN A 153 45.804 70.420 27.145 1.00 33.22 ATOM 985 CB GEN A 153 44.401 72.448 29.144 1.00 33.22 ATOM 986 CG GEN A 153 44.600 73.376 30.557 1.00 32.53 ATOM 987 CD GEN A 153 44.600 73.376 30.557 1.00 32.73 ATOM 988 OEI GEN A 153 43.301 73.649 31.122 1.00 30.78 ATOM 989 NEZ GEN A 153 43.301 73.649 31.122 1.00 30.78 ATOM 999 N TRP A 154 44.658 71.838 25.883 1.00 32.73 ATOM 991 CA TRP A 154 44.658 71.838 25.883 1.00 32.73 ATOM 993 O TRP A 154 44.553 70.907 24.769 1.00 33.13 ATOM 995 CG TRP A 154 44.551 70.907 24.769 1.00 33.13 ATOM 995 CG TRP A 154 44.551 70.907 24.769 1.00 33.13 ATOM 995 CG TRP A 154 44.551 70.907 24.769 1.00 33.13 ATOM 995 CG TRP A 154 44.551 70.907 24.769 1.00 33.13 ATOM 996 CG TRP A 154 44.551 70.907 24.769 1.00 33.13 ATOM 997 CG TRP A 154 44.551 70.907 24.769 1.00 33.13 ATOM 998 CG TRP A 154 44.551 70.907 24.769 1.00 33.13 ATOM 998 CG TRP A 154 44.551 70.907 24.769 1.00 35.24 ATOM 998 CG TRP A 154 44.551 70.907 24.769 1.00 35.24 ATOM 998 CG TRP A 154 44.551 7	5	ATOM ATOM	972 973	CG OD: ND:	ASN 1 ASN 2 ASN	A 151 A 151 A 151	49.484 50.396 49.486	79.088 78.429 80.411	31.515 32.016 31.508	1.00 40.94 1.00 47.50 1.00 39.57
ATOM 980 CG2 THR A 152 45.978 77.550 25.079 1.00 34.93 ATOM 981 N GLN A 153 45.461 73.960 27.524 1.00 32.33 ATOM 982 CG GLN A 153 45.461 73.960 27.524 1.00 32.33 ATOM 983 C GLN A 153 45.461 73.960 27.524 1.00 32.33 ATOM 983 C GLN A 153 45.461 70.3960 27.524 1.00 32.33 ATOM 984 O GLN A 153 45.333 71.526 26.970 1.00 32.33 ATOM 985 CB GLN A 153 45.333 71.526 26.970 1.00 32.33 ATOM 986 CG GLN A 153 45.333 71.526 26.970 1.00 32.33 ATOM 986 CG GLN A 153 45.301 70.342 27.145 1.00 33.22 ATOM 986 CG GLN A 153 44.600 73.376 30.357 1.00 29.66 ATOM 987 CD GLN A 153 44.600 73.376 30.357 1.00 29.66 ATOM 988 NE2 GLN A 153 43.301 73.649 31.122 1.00 30.78 ATOM 989 NE2 GLN A 153 43.192 73.112 32.339 1.00 28.57 ATOM 990 N TRP A 154 44.653 70.907 24.769 1.00 32.73 ATOM 990 C TRP A 154 44.553 70.907 24.769 1.00 33.13 ATOM 993 O TRP A 154 44.181 71.690 23.557 1.00 32.74 ATOM 997 CD TRP A 154 43.483 69.853 24.982 1.00 32.74 ATOM 999 C C TRP A 154 43.483 69.853 24.982 1.00 32.74 ATOM 999 C CD TRP A 154 43.483 69.853 24.982 1.00 32.74 ATOM 999 C CD TRP A 154 43.483 69.853 24.982 1.00 32.74 ATOM 999 C CD TRP A 154 43.483 69.853 24.982 1.00 36.41 ATOM 999 C CD TRP A 154 44.651 67.895 23.497 1.00 31.33 ATOM 996 CD TRP A 154 44.651 67.806 23.672 1.00 32.74 ATOM 999 C CD TRP A 154 44.651 67.806 23.672 1.00 32.74 ATOM 000 CC2 TRP A 154 44.6570 66.160 21.735 1.00 36.52 ATOM 1000 CC2 TRP A 154 44.555 67.479 24.056 1.00 34.17 ATOM 1000 CC2 TRP A 154 44.5570 66.160 21.735 1.00 36.52 ATOM 1001 CC2 TRP A 154 44.555 67.479 22.298 1.00 36.41 ATOM 1000 CC2 TRP A 154 44.5570 66.160 21.735 1.00 36.52 ATOM 1000 CC2 TRP A 154 44.5570 66.160 21.735 1.00 36.52 ATOM 1001 CC2 TRP A 154 44.5570 66.160 21.735 1.00 36.52 ATOM 1001 CC2 TRP A 154 44.6570 66.160 21.735 1.00 35.50 ATOM 1001 CC2 TRP A 154 44.6570 66.160 21.735 1.00 35.50 ATOM 1001 CC2 TRP A 156 44.687 1.264 22.403 1.00 36.50 ATOM 1002 CC TRP A 156 44.689 77.752 1.00 31.50 3.00 ATOM 1003 CR TRP A 157 44.680 77.752 1.00 31.30 3.00 ATOM 1003 CR TRP A 157 44.680 77.75	10	ATOM ATOM ATOM	976 977 978	C O CB	THR THR THR	A 152 A 152 A 152	46.381 46.579 47.716	76.084 74.644 74.159	26.917 27.290 27.346	1.00 34.29 1.00 33.28 1.00 32.47
ATOM 984 O GLN A 153 45.804 70.420 77.145 1.00 33.22 ATOM 985 CB G GLN A 153 44.401 72.448 29.144 1.00 31.84 ATOM 987 CD GLN A 153 44.600 73.376 30.357 1.00 29.66 ATOM 988 OEI GLN A 153 42.395 74.320 30.598 1.00 29.68 ATOM 989 NE2 GLN A 153 42.395 74.320 30.598 1.00 29.78 ATOM 989 NE2 GLN A 153 42.395 74.320 30.598 1.00 29.78 ATOM 989 NE2 GLN A 153 42.395 74.320 30.598 1.00 32.52 ATOM 9910 N TRF A 154 44.658 71.838 25.883 1.00 32.73 ATOM 9910 CA TRF A 154 44.553 70.907 24.769 1.00 33.07 ATOM 992 C TRF A 154 44.553 70.907 24.769 1.00 33.07 ATOM 993 O TRF A 154 44.553 70.907 24.769 1.00 33.07 ATOM 994 CB TRF A 154 43.471 71.690 23.557 1.00 32.32 ATOM 995 CG TRF A 154 43.471 71.690 23.557 1.00 32.32 ATOM 995 CG TRF A 154 43.471 71.690 23.557 1.00 32.32 ATOM 995 CD TRF A 154 43.471 71.690 23.557 1.00 32.32 ATOM 995 CD TRF A 154 43.471 71.690 23.557 1.00 32.32 ATOM 995 CD TRF A 154 43.483 69.853 24.982 1.00 32.428 ATOM 999 CD TRF A 154 44.351 67.895 23.497 1.00 36.428 ATOM 999 CD TRF A 154 44.555 67.896 22.008 1.00 36.83 ATOM 999 CD TRF A 154 44.555 67.896 22.008 1.00 35.24 ATOM 1000 CE3 TRF A 154 44.555 67.490 22.293 1.00 36.83 ATOM 1000 CE3 TRF A 154 44.570 67.806 22.008 1.00 35.77 ATOM 1000 CE3 TRF A 154 44.570 67.806 22.008 1.00 35.77 ATOM 1000 CE3 TRF A 154 44.570 67.222 22.353 1.00 36.83 ATOM 1000 CC2 TRF A 154 44.570 65.774 22.298 1.00 37.72 ATOM 1000 CC2 TRF A 154 44.570 65.774 22.298 1.00 37.72 ATOM 1000 CC2 TRF A 154 44.570 65.774 22.298 1.00 36.86 ATOM 1001 CC2 TRF A 154 46.624 66.415 23.452 1.00 37.72 ATOM 1002 CC3 TRF A 154 46.624 66.415 23.452 1.00 36.93 ATOM 1005 CA VAL A 155 44.682 71.264 22.403 1.00 36.86 ATOM 1007 O VALA 155 44.682 71.264 22.403 1.00 36.502 ATOM 1008 CB VAL A 155 44.970 70.31 20.105 1.00 35.02 ATOM 1008 CB VAL A 155 44.970 70.31 20.105 1.00 35.30 ATOM 1008 CB VAL A 155 44.970 70.31 20.105 1.00 35.30 ATOM 1008 CB VAL A 155 44.970 70.31 20.105 1.00 35.30 ATOM 1002 CC VAL A 155 44.970 70.31 20.105 1.00 35.30 ATOM 1002 CC VAL A 155 44.970 70.31 20.105 1.00 35.30 ATOM 1003 CRE VAL A 155	15	ATOM ATOM ATOM	980 981 982	CG2 N CA	GLN GLN	A 152 A 153 A 153	45.440 45.461 45.485	75.341 73.960 72.602	24.767 27.524 28.045	1.00 34.46 1.00 34.93 1.00 32.18 1.00 32.33
ATOM 989 NEZ GLN A 153 43.192 73.112 32.339 1.00 28.52 ATOM 991 CA TRP A 154 44.658 71.838 25.839 1.00 32.73 ATOM 992 C TRP A 154 44.553 70.907 24.769 1.00 33.07 ATOM 993 O TRP A 154 44.553 70.907 24.769 1.00 33.07 ATOM 993 C TRP A 154 43.471 72.646 23.672 1.00 32.32 ATOM 995 CG TRP A 154 43.471 72.646 23.672 1.00 32.32 ATOM 995 CG TRP A 154 43.499 68.893 24.982 1.00 34.28 ATOM 996 CD1 TRP A 154 43.499 68.807 22.899 1.00 36.41 ATOM 997 CD2 TRP A 154 44.551 67.895 23.497 1.00 34.28 ATOM 999 CE2 TRP A 154 44.551 67.895 23.497 1.00 34.65 ATOM 999 CE2 TRP A 154 43.867 67.222 22.351 1.00 36.24 ATOM 1000 CE3 TRP A 154 44.551 67.895 23.497 1.00 34.65 ATOM 1001 C22 TRP A 154 44.570 66.160 21.731 1.00 36.92 ATOM 1002 CA VAL A 155 44.682 71.264 22.403 1.00 36.92 ATOM 1004 N VAL A 155 44.682 71.264 22.403 1.00 34.38 ATOM 1005 CA VAL A 155 44.682 71.264 22.403 1.00 36.30 ATOM 1006 C VAL A 155 44.890 73.635 19.468 1.00 34.58 ATOM 1007 O VAL A 155 44.890 73.635 19.468 1.00 34.58 ATOM 1009 CGI VAL A 155 44.890 73.635 19.468 1.00 34.58 ATOM 1009 CGI VAL A 155 44.890 73.635 19.468 1.00 35.30 ATOM 1010 CG2 VAL A 155 44.890 73.635 19.468 1.00 36.54 ATOM 1010 CG2 VAL A 155 44.890 73.635 19.468 1.00 36.58 ATOM 1010 CG2 VAL A 155 44.890 73.635 19.468 1.00 35.30 ATOM 1010 CG2 VAL A 155 44.890 73.635 19.468 1.00 36.58 ATOM 1010 CG2 VAL A 155 44.890 73.635 19.468 1.00 35.30 ATOM 1010 CG2 VAL A 155 44.890 73.635 19.468 1.00 35.30 ATOM 1010 CG2 VAL A 155 45.443 72.731 20.565 1.00 35.30 ATOM 1010 CG2 VAL A 155 45.443 72.731 20.565 1.00 35.30 ATOM 1010 CG2 VAL A 155 46.090 73.548 21.664 1.00 38.86 ATOM 1010 CG2 VAL A 155 46.090 73.548 21.667 1.00 35.68 ATOM 1010 CG2 VAL A 155 46.090 73.548 21.667 1.00 35.59 ATOM 1010 CG2 VAL A 155 46.090 73.548 21.667 1.00 35.59 ATOM 1010 CG2 VAL A 155 46.090 73.548 21.667 1.00 35.59 ATOM 1010 CG2 VAL A 155 46.090 73.548 21.667 1.00 35.59 ATOM 1020 CC2 TRP A 157 46.003 70.529 11.003 35.50 ATOM 1010 CG2 VAL A 155 46.090 73.548 21.667 1.00 35.59 ATOM 1021 CC2 TRP A 157 46.	20	ATOM ATOM ATOM ATOM	984 985 986 987	O CB CG CD	GLN A GLN A GLN A	A 153 A 153 A 153 A 153	45.804 44.401 44.600 43.301	70.420 72.448 73.376 73.649	27.145 29.144 30.357 31.122	1.00 33.22 1.00 31.84 1.00 29.66 1.00 30.78
ATOM 994 CB TRP A 154 43.471 72.646 23.672 1.00 32.32 ATOM 995 CG TRP A 154 43.483 69.853 24.982 1.00 32.74 ATOM 996 CD1 TRP A 154 42.403 68.807 22.899 1.00 34.28 ATOM 996 CD1 TRP A 154 42.403 68.807 22.899 1.00 34.28 ATOM 998 CD2 TRP A 154 44.351 67.895 23.497 1.00 34.65 ATOM 998 NEI TRP A 154 44.351 67.895 23.497 1.00 34.65 ATOM 998 NEI TRP A 154 42.675 67.806 22.008 1.00 34.17 ATOM 998 CD2 TRP A 154 42.675 67.806 22.008 1.00 34.17 ATOM 1000 CE3 TRP A 154 45.555 67.479 24.056 1.00 34.17 ATOM 1001 C22 TRP A 154 45.555 67.479 24.056 1.00 34.17 ATOM 1002 CZ3 TRP A 154 45.555 67.479 24.056 1.00 34.17 ATOM 1004 N VAL A 155 44.682 71.264 22.403 1.00 36.01 ATOM 1004 N VAL A 155 44.682 71.264 22.403 1.00 36.01 ATOM 1005 CA VAL A 155 44.682 71.264 22.403 1.00 34.39 ATOM 1005 CA VAL A 155 44.928 69.760 20.138 1.00 34.58 ATOM 1008 CB VAL A 155 44.928 69.760 20.138 1.00 36.33 ATOM 1008 CB VAL A 155 44.928 69.760 20.138 1.00 36.35 ATOM 1009 CG1 VAL A 155 44.928 69.760 20.138 1.00 36.35 ATOM 1010 CC2 VAL A 155 44.928 69.760 20.138 1.00 36.34 ATOM 1010 CC2 VAL A 155 44.928 69.760 20.138 1.00 36.34 ATOM 1010 CC2 VAL A 155 44.928 69.760 20.138 1.00 36.34 ATOM 1010 CC2 VAL A 155 44.928 69.760 20.138 1.00 36.34 ATOM 1010 CC2 VAL A 155 44.928 69.760 20.138 1.00 36.35 ATOM 1011 N THR A 156 43.222 70.873 19.193 1.00 34.458 ATOM 1011 N THR A 156 42.296 67.767 17.476 1.00 35.30 ATOM 1012 CA THR A 156 42.296 67.767 17.476 1.00 35.521 ATOM 1013 C THR A 156 42.256 67.767 17.476 1.00 35.559 ATOM 1018 N TRP A 157 42.562 70.616 14.411 1.00 36.38 ATOM 1010 CC3 TRP A 157 44.564 70.731 12.3161 1.00 35.59 ATOM 1023 CG TRP A 157 44.754 71.01 33.216 1.00 35.55 ATOM 1024 CD TRP A 157 44.754 71.01 33.216 1.00 35.55 ATOM 1025 CD2 TRP A 157 44.754 71.01 33.216 1.00 35.55 ATOM 1024 CD TRP A 157 44.754 71.01 33.216 1.00 35.55 ATOM 1025 CD2 TRP A 157 44.754 71.01 33.216 1.00 35.55 ATOM 1026 CD2 TRP A 157 44.754 71.01 33.216 1.00 35.55 ATOM 1027 CD2 TRP A 157 44.754 71.01 33.216 1.00 35.55 ATOM 1026 CD2 TRP A 157 44.769 70.240 13.223 1.00 35.55 ATOM 10	25	ATOM ATOM ATOM	989 990 991 992	NE2 N CA	GLN I TRP I TRP I	A 153 A 154 A 154 A 154	43.192 44.658 44.553	73.112 71.838 70.907	32.339 25.883 24.769	1.00 28.52 1.00 32.73 1.00 33.07
ATOM 999 CE2 TRP A 154 43.867 67.222 22.353 1.00 36.83 ATOM 1000 CE3 TRP A 154 45.555 67.479 24.056 1.00 34.17 35 ATOM 1001 CZ2 TRP A 154 44.5770 66.160 21.735 1.00 36.92 ATOM 1002 CZ3 TRP A 154 44.5770 66.160 21.735 1.00 36.92 ATOM 1003 CH2 TRP A 154 46.248 66.415 23.452 1.00 37.72 ATOM 1001 CZ2 TRP A 154 46.248 66.415 23.452 1.00 37.72 ATOM 1004 N VAL A 155 44.682 71.264 22.298 1.00 36.01 ATOM 1005 CA VAL A 155 44.682 71.264 22.298 1.00 36.01 ATOM 1006 C VAL A 155 44.682 71.264 22.403 1.00 34.39 ATOM 1006 C VAL A 155 44.176 70.731 20.105 1.00 35.30 ATOM 1008 CB VAL A 155 44.928 69.760 20.138 1.00 34.58 ATOM 1009 CG1 VAL A 155 44.890 73.635 19.468 1.00 36.34 ATOM 1010 CG2 VAL A 155 44.890 73.635 19.468 1.00 36.34 ATOM 1010 CG2 VAL A 155 44.890 73.635 19.468 1.00 36.34 ATOM 1011 N THR A 156 43.222 70.873 19.193 1.00 34.41 ATOM 1012 CA THR A 156 43.222 70.873 19.193 1.00 34.462 ATOM 1013 C THR A 156 42.509 70.539 16.891 1.00 35.60 ATOM 1015 CB THR A 156 42.256 67.767 17.476 1.00 35.50 ATOM 1017 CC2 THR A 156 42.226 67.767 17.476 1.00 35.59 ATOM 1017 CC2 THR A 156 42.226 67.767 17.476 1.00 35.59 ATOM 1017 CC2 THR A 156 42.226 67.767 17.476 1.00 35.59 ATOM 1017 CC2 THR A 156 42.226 67.767 17.476 1.00 35.59 ATOM 1017 CC2 THR A 156 42.226 67.767 17.476 1.00 35.55 ATOM 1020 C TRP A 157 43.124 70.231 15.704 1.00 35.581 ATOM 1020 C TRP A 157 43.124 70.231 15.704 1.00 35.80 ATOM 1020 C TRP A 157 44.554 70.231 15.704 1.00 35.80 ATOM 1022 CB TRP A 157 44.554 71.013 13.266 1.00 35.35 ATOM 1022 CB TRP A 157 44.564 71.013 13.266 1.00 35.35 ATOM 1022 CB TRP A 157 44.564 71.013 13.266 1.00 35.35 ATOM 1022 CB TRP A 157 44.863 72.388 12.847 1.00 33.33 ATOM 1022 CD TRP A 157 44.863 72.388 12.847 1.00 33.33 ATOM 1022 CD TRP A 157 44.863 72.388 12.847 1.00 33.33 ATOM 1022 CD TRP A 157 44.863 72.388 12.847 1.00 33.33 ATOM 1022 CD TRP A 157 44.863 72.388 12.847 1.00 33.33 ATOM 1022 CD TRP A 157 44.927 12.255 1.00 36.86 ATOM 1030 CZ3 TRP A 157 44.927 12.255 1.00 33.33 ATOM 1024 CD1 TRP A 157 44.927 12.255 1.00 33.386 ATOM 1034 CS CZ2	30	ATOM ATOM ATOM ATOM	994 995 996 997	CB CG CD1 CD2	TRP ATRP ATRP A	A 154 A 154 A 154 A 154	43.483 43.399 42.403 44.351	69.853 68.894 68.807 67.895	23.672 24.982 23.838 22.899 23.497	1.00 32.32 1.00 32.74 1.00 34.28 1.00 36.41 1.00 34.65
ATOM 1004 N VAL A 155	35	ATOM ATOM ATOM ATOM	999 1000 1001 1002	CE2 CE3 CZ2 CZ3	TRP ATRP ATRP A	154 154 154 154	43.867 45.555 44.570 46.248	67.222 67.479 66.160 66.415	22.353 24.056 21.735	1.00 36.83 1.00 34.17 1.00 36.92
ATOM 1008 CB VAL A 155	40	ATOM ATOM ATOM	1004 1005 1006	N CA C	VAL A VAL A	155 155 155	44.682 44.330 44.176	71.264 71.845 70.731	22.403 21.127 20.105	1.00 34.39 1.00 35.30 1.00 35.02
ATOM 1013 C THR A 156	45	ATOM ATOM ATOM	1009 1010 1011	CG1 CG2 N	VAL A VAL A THR A	155 155 156	45.443 44.890 46.090 43.222	72.731 73.635 73.548 70.873	20.562 19.468 21.654 19.193	1.00 35.77 1.00 36.34 1.00 38.86 1.00 34.41
ATOM 1018 N TRP A 157 43.124 70.231 15.704 1.00 35.68 ATOM 1019 CA TRP A 157 42.562 70.616 14.411 1.00 36.30 ATOM 1020 C TRP A 157 41.330 69.778 14.186 1.00 36.28 ATOM 1021 O TRP A 157 41.235 68.679 14.687 1.00 35.81 ATOM 1022 CB TRP A 157 43.507 70.240 13.263 1.00 36.56 ATOM 1023 CG TRP A 157 44.754 71.013 13.176 1.00 35.29 ATOM 1024 CD1 TRP A 157 46.003 70.555 13.352 1.00 35.35 ATOM 1025 CD2 TRP A 157 44.863 72.388 12.847 1.00 33.33 60 ATOM 1026 NE1 TRP A 157 46.910 71.572 13.161 1.00 36.83 ATOM 1028 CE3 TRP A 157 46.224 72.703 12.817 1.00 33.51 ATOM 1028 CE3 TRP A 157 46.678 73.976 12.563 1.00 32.60 ATOM 1029 CZ2 TRP A 157 44.391 74.628 12.233 1.00 30.65 ATOM 1030 CZ3 TRP A 157 44.391 74.628 12.233 1.00 30.65 ATOM 1031 CH2 TRP A 157 45.741 74.927 12.265 1.00 30.48 ATOM 1032 N SER A 158 40.407 70.290 13.404 1.00 37.62 ATOM 1033 CA SER A 158 39.260 69.503 12.980 1.00 38.44 ATOM 1034 C SER A 158 39.858 68.436 12.063 1.00 39.22 ATOM 1035 O SER A 158 39.858 68.436 12.063 1.00 39.22 ATOM 1035 O SER A 158 39.858 68.436 12.063 1.00 39.22 ATOM 1035 O SER A 158 41.005 68.554 11.675 1.00 38.90	50	ATOM ATOM ATOM ATOM	1013 1014 1015 1016	C O CB OG1	THR A THR A THR A	156 156 156 156	42.509 41.553 42.328 42.256	70.539 71.308 68.675 67.767	16.853 16.919 18.567 17.476	1.00 35.68 1.00 34.62 1.00 35.21 1.00 37.50
ATOM 1023 CG TRP A 157 44.754 71.013 13.176 1.00 35.29 ATOM 1024 CD1 TRP A 157 46.003 70.555 13.352 1.00 35.35 ATOM 1025 CD2 TRP A 157 44.863 72.388 12.847 1.00 33.33 ATOM 1026 NEI TRP A 157 46.910 71.572 13.161 1.00 36.83 ATOM 1027 CE2 TRP A 157 46.910 71.572 13.161 1.00 33.51 ATOM 1028 CE3 TRP A 157 43.940 73.385 12.530 1.00 32.60 ATOM 1029 CZ2 TRP A 157 46.678 73.976 12.563 1.00 32.88 ATOM 1030 CZ3 TRP A 157 46.678 73.976 12.563 1.00 32.88 ATOM 1031 CH2 TRP A 157 44.391 74.628 12.233 1.00 30.65 ATOM 1032 N SER A 158 40.407 70.290 13.404 1.00 37.62 ATOM 1033 CA SER A 158 39.260 69.503 12.980 1.00 38.44 ATOM 1034 C SER A 158 39.858 68.436 12.063 1.00 39.22 ATOM 1035 O SER A 158 41.005 68.554 11.675 1.00 38.90	55	ATOM ATOM ATOM ATOM	1018 1019 1020 1021	N CA C O	TRP A TRP A TRP A	157 157 157 157	43.124 42.562 41.330 41.235	70.231 70.616 69.778 68.679	15.704 14.411 14.186 14.687	1.00 35.68 1.00 36.30 1.00 36.28 1.00 35.81
ATOM 1028 CE3 TRP A 157 43.940 73.385 12.530 1.00 32.60 ATOM 1029 CZ2 TRP A 157 46.678 73.976 12.563 1.00 32.88 ATOM 1030 CZ3 TRP A 157 44.391 74.628 12.233 1.00 30.65 ATOM 1031 CH2 TRP A 157 45.741 74.927 12.265 1.00 30.48 ATOM 1032 N SER A 158 40.407 70.290 13.404 1.00 37.62 ATOM 1033 CA SER A 158 39.260 69.503 12.980 1.00 38.44 ATOM 1034 C SER A 158 39.858 68.436 12.063 1.00 39.22 ATOM 1035 O SER A 158 41.005 68.554 11.675 1.00 38.90	60	ATOM ATOM ATOM ATOM	1023 1024 1025 1026	CG CD1 CD2 NE1	TRP A TRP A TRP A	157 157 157 157	44.754 46.003 44.863 46.910	71.013 70.555 72.388 71.572	13.176 13.352 12.847 13.161	1.00 35.29 1.00 35.35 1.00 33.33 1.00 36.83
ATOM 1033 CA SER A 158 39.260 69.503 12.980 1.00 38.44 ATOM 1034 C SER A 158 39.858 68.436 12.063 1.00 39.22 ATOM 1035 O SER A 158 41.005 68.554 11.675 1.00 38.90	65	ATOM ATOM ATOM ATOM	1028 1029 1030 1031	CE3 CZ2 CZ3 CH2	TRP A TRP A TRP A	157 157 157 157	43.940 46.678 44.391 45.741	73.385 73.976 74.628 74.927	12.530 12.563 12.233 12.265	1.00 32.60 1.00 32.88 1.00 30.65 1.00 30.48
1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	70	MOTA MOTA MOTA	1033 1034 1035	CA C O	SER A SER A SER A	158 158 158	39.260 39.858 41.005	69.503 68.436	12.980 12.063	1.00 38.44 1.00 39.22

	ATOM	1037	OG	SER A	158	38.943	71.285	11.441	1.00	36.37
						39.127	67.384	11.736	1.00	
	MOTA	1038	N	PRO A						
	ATOM	1039	CA	PRO A		39.745	66.256	11.014	1.00	
	ATOM	1040	С	PRO A	159	40.010	66.532	9.552	1.00	44.36
5	ATOM	1041	0	PRO A	159	40.795	65.810	8.942	1.00	45.26
_	ATOM	1042	CB	PRO A		38.708	65.138	11.103	1.00	42.08
		1042		PRO A		37.607	65.652	11.896		42.11
	ATOM		CG							
	ATOM	1044	CD	PRO A		37.709	67.164	11.985		40.54
	ATOM	1045	N	VAL A		39.383	67.558	9.004	1.00	
10	ATOM	1046	CA	VAL A	160	39.487	67.800	7.592	1.00	47.33
	ATOM	1047	С	VAL A	160	39.335	69.255	7.251	1.00	47.02
	ATOM	1048	ŏ	VAL A		38.227	69.687	6.981	1.00	48.15
		1049		VAL A		38.351	67.046	6.891		48.20
	ATOM		CB							
	ATOM	1050		VAL A		37.857	67.793	5.706		48.33
15	ATOM	1051	CG2	VAL A	160	38.803	65.639	6.499		49.68
	ATOM	1052	N	GLY A	161	40.428	70.010	7.237	1.00	45.77
	ATOM	1053	CA	GLY A	161	40.341	71.439	6.972	1.00	44.86
	ATOM	1054	C	GLY A		41.305	72.178	7.886	1.00	
		1055		GLY A		42.466	71.822	7.964		42.53
••	ATOM		0							
20	ATOM	1056	N	HIS A		40.850	73.220	8.566		42.39
	ATOM	1057	CA	HIS A	162	41.748	73.892	9.512		41.52
	ATOM	1058	С	HIS A	162	41.047	74.636	10.666	1.00	40.24
	ATOM	1059	0	HIS A	162	41.517	75.654	11.123	1.00	38.94
	ATOM	1060	ČВ	HIS A		42.699	74.805	8.752	1.00	41.07
25		1061		HIS A		42.007	75.869	7.976		42.04
25 -	ATOM		CG					6.611		
	MOTA	1062		HIS A		42.150	76.002			43.01
	ATOM	1063		HIS A		41.174	76.861	8.371		42.61
	ATOM	1064	CE1	HIS A	162	41.416	77.022	6.199	1.00	44.93
	ATOM	1065	NE2	HIS A	162	40.813	77.559	7.248	1.00	43.01
30	ATOM	1066	N	LYS A		39.900	74.139	11.101	1.00	40.02
50	ATOM	1067	CA	LYS A		39.255	74.668	12.297		39.80
										39.23
	ATOM	1068	C	LYS A		40.092	74.243	13.507		
	MOTA	1069	0	LYS A		40.831	73.277	13.436		39.27
	MOTA	1070	CB	LYS A	163	37.825	74.133	12.427	1.00	40.08
35	ATOM	1071	CG	LYS A	163	36.841	74.602	11.337	1.00	41.67
	ATOM	1072	CD	LYS A		35.389	74.250	11.717	1.00	43.49
	ATOM	1073	CE	LYS A		34.377	74.600	10.604		45.24
						33.021	74.073	10.922		44.53
	ATOM	1074	NZ	LYS A						
	ATOM	1075	N	LEU A		40.002	74.984	14.612		38.88
40	ATOM	1076	CA	LEU A	164	40.754	74.659	15.817	1.00	38.35
	ATOM	1077	С	LEU A	164	39.831	74.614	17.021	1.00	37.44
	ATOM	1078	0	LEU A	164	38.947	75.453	17.144	1.00	37.74
	ATOM	1079	ČВ	LEU A		41.819	75.723	16.098		38.44
	ATOM	1080	CG	LEU A		43.153	75.629	15.373	1.00	39.70
45						43.133	76.881		1.00	40.58
45	ATOM	1081		LEU A				15.604		
	ATOM	1082	CD2	LEU A		43.939	74.433	15.817		39.25
	ATOM	1083	N	ALA A	165	40.040	73.641	17.909	1.00	36.10
	ATOM	1084	CA	ALA A	165	39.347	73.630	19.184	1.00	35.22
	ATOM	1085	С	ALA A	165	40.381	73.531	20.277	1.00	34.55
50	ATOM	1086	ō	ALA A		41.298	72.755	20.204		33.31
50				ALA A		38.310	72.508	19.289		34.85
	ATOM	1087	CB							
	MOTA	1088	N	TYR A		40.234	74.337	21.311		34.62
	ATOM	1089	CA	TYR A		41.186	74.283	22.397		33.94
	ATOM	1090	С	TYR A	166	40.522	74.510	23.727	1.00	33.50
55	ATOM	1091	0	TYR A		39.417	75.045	23.809	1.00	31.59
	ATOM	1092	СВ	TYR A		42.299	75.291	22.179	1.00	34.14
				TYR A		41.868	76.728	22.206		36.02
	ATOM	1093	CG							
	ATOM	1094	CD1			41.811	77.419	23.410		38.52
	MOTA	1095	CD2	TYR A		41.585	77.417	21.045		38.10
60	ATOM	1096	CE1	TYR A	166	41.470	78.729	23.473		38.65
	ATOM	1097	CE2	TYR A		41.245	78.775	21.097	1.00	39.86
	ATOM	1098	CZ	TYR A		41.184	79.413	22.335		38.33
										35.71
	MOTA	1099	OH	TYR A		40.824	80.725	22.463		
	ATOM	1100	N	VAL A		41.248	74.105	24.767		33.32
65	ATOM	1101	CA	VAL A		40.771	74.134	26.123		33.62
	ATOM	1102	С	VAL A	167	41.739	74.941	26.943		34.02
	ATOM	1103	Ō	VAL A		42.924	74.627	26.996		33.50
	ATOM	1104	СВ	VAL A		40.723	72.732	26.689		33.48
	ATOM	1104		VAL A		40.723	72.763	28.202		33.98
70										
70	ATOM	1106	CG2	VAL A	101	39.737	71.916	25.934	1.00	34.69

	MOTA MOTA MOTA	1107 N 1108 C 1109 C	TRP A 168 A TRP A 168 TRP A 168	41.212 41.988 41.126	3 76.887	28.405	1.00 35.04
5	ATOM	1110 O 1111 CE 1112 CG	TRP A 168 3 TRP A 168	39.932 42.292 43.055	77.500 78.150 79.241	29.487 27.603 28.346	1.00 34.71 1.00 35.59 1.00 37.17
10	ATOM ATOM ATOM ATOM	1114 CT 1115 NE 1116 CE 1117 CE	D2 TRP A 168 C1 TRP A 168 C2 TRP A 168 C3 TRP A 168	44.354 42.547 44.695 43.596 41.310	80.506 80.380 81.195	28.752 29.353 29.387	1.00 38.52 1.00 39.17 1.00 41.72
15	ATOM ATOM ATOM ATOM ATOM	1119 CZ	22 TRP A 168 3 TRP A 168 42 TRP A 168 ASN A 169 ASN A 169	43.444 41.152 42.213 41.711	82.489 82.414 83.073 77.079	29.912 29.179 29.796 30.811	1.00 43.72 1.00 44.45 1.00 43.32 1.00 34.34
20	ATOM ATOM ATOM ATOM	1123 C 1124 O 1125 CB 1126 CG	ASN A 169 ASN A 169 ASN A 169 ASN A 169	40.989 39.729 38.691 40.688 41.888	76.453 76.851 78.805 79.576	32.045 32.119 32.618 32.210 32.756	1.00 34.21 1.00 33.09 1.00 30.84 1.00 34.41 1.00 38.60
25	ATOM ATOM ATOM ATOM ATOM		1 ASN A 169 2 ASN A 169 ASN A 170 ASN A 170 ASN A 170	41.801 43.012 39.862 38.842 37.615	78.882 75.244 74.219	33.014 32.954 31.596 31.682 30.844	1.00 44.54 1.00 39.87 1.00 32.83 1.00 32.10 1.00 31.06
30	ATOM ATOM ATOM ATOM ATOM	1132 O 1133 CB 1134 CG 1135 OD	ASN A 170 ASN A 170 ASN A 170 1 ASN A 170	36.624 38.462 39.577 40.751	73.782 73.971 73.286 73.469	31.001 33.153 33.945 33.679	1.00 30.55 1.00 32.85 1.00 33.35 1.00 34.79
30	ATOM ATOM ATOM ATOM	1136 ND2 1137 N 1138 CA 1139 C 1140 O	2 ASN A 170 ASP A 171 ASP A 171 ASP A 171 ASP A 171	39.192 37.664 36.562 37.013 38.167	72.515 75.460 75.684 75.482 75.659	34.937 29.948 29.005 27.535 27.190	1.00 32.85 1.00 31.17 1.00 31.06 1.00 30.59 1.00 30.25
35	ATOM ATOM ATOM ATOM ATOM	1144 OD2	ASP A 171 ASP A 171 L ASP A 171 2 ASP A 171	35.993 35.138 34.224 35.321	77.097 77.270 76.431 78.238	29.148 30.383 30.664 31.125	1.00 31.19 1.00 31.15 1.00 29.15 1.00 30.82
40	ATOM ATOM ATOM ATOM	1145 N 1146 CA 1147 C 1148 O 1149 CB	ILE A 172 ILE A 172 ILE A 172 ILE A 172 ILE A 172	36.067 36.339 36.173 35.215 35.385	75.147 74.932 76.191 76.910 73.882	26.673 25.264 24.444 24.627 24.724	1.00 30.17 1.00 30.16 1.00 30.54 1.00 30.37
45	ATOM ATOM ATOM ATOM	1150 CG1 1151 CG2 1152 CD1 1153 N	ILE A 172 LILE A 172	35.615 35.583 34.434 37.127	73.882 72.570 73.729 71.624 76.456	24.724 25.450 23.235 25.459 23.563	1.00 29.51 1.00 27.93 1.00 30.53 1.00 29.06 1.00 31.38
50	ATOM ATOM ATOM ATOM ATOM	1154 CA 1155 C 1156 O 1157 CB 1158 CG	TYR A 173 TYR A 173 TYR A 173 TYR A 173 TYR A 173	37.010 37.193 37.876 38.037	77.526 76.928 75.901 78.633	22.590 21.181 21.016 22.833	1.00 33.28 1.00 34.60 1.00 33.51 1.00 33.55
55	ATOM ATOM ATOM ATOM ATOM	1159 CD1 1160 CD2 1161 CE1	TYR A 173 TYR A 173 TYR A 173 TYR A 173 TYR A 173	37.867 38.130 37.415 37.972 37.236	79.289 78.577 80.602 79.160 81.198	24.189 25.344 24.311 26.609 25.571	1.00 33.93 1.00 35.75 1.00 32.65 1.00 37.59 1.00 34.72
60	ATOM ATOM ATOM ATOM	1164 OH 1165 N 1166 CA 1167 C	TYR A 173 VAL A 174 VAL A 174 VAL A 174	37.524 37.352 36.570 36.677 37.133	80.474 81.009 77.572 77.154 78.311	26.711 27.965 20.190 18.813 17.940	1.00 36.29 1.00 36.67 1.00 35.32 1.00 36.57 1.00 37.79
65	ATOM ATOM ATOM ATOM ATOM		VAL A 174 VAL A 174 VAL A 174 VAL A 174 LYS A 175	36.676 35.329 35.462 34.851 37.998	79.424 76.696 76.409 75.474 78.016	18.108 18.249 16.776 18.945	1.00 38.26 1.00 36.38 1.00 37.71 1.00 36.20
70	ATOM ATOM ATOM ATOM	1173 CA 1174 C 1175 O 1176 CB	LYS A 175 LYS A 175 LYS A 175 LYS A 175 LYS A 175	38.463 38.191 38.711 39.958	78.984 78.463 77.420 79.225	16.979 15.998 14.599 14.191 16.131	1.00 39.34 1.00 40.41 1.00 40.91 1.00 40.44 1.00 41.02

	ATOM	1177	CG	LYS A	175	40.310	80.403	17.018	1.00	42.53
	ATOM	1178	CD	LYS A		41.728	80.325	17.482		43.95
	ATOM	1179	CE	LYS A		42.378	81.679	17.502		45.63
	ATOM	1180	NZ	LYS A		42.799	82.132	16.146	1.00	
5	ATOM	1181	N	ILE A	176	37.372	79.209	13.870	1.00	41.50
	ATOM	1182	CA	ILE A	176	37.026	78.879	12.506	1.00	41.87
	ATOM	1183	C	ILE A		38.245	79.118	11.636	1.00	42.08
	ATOM	1184	ŏ	ILE A		38.622	78.269	10.867		41.73
						35.829	79.699	12.080		42.04
• •	ATOM	1185	CB	ILE A						
10	ATOM	1186	CG1			34.653	79.349	12.992		43.27
	ATOM	1187	CG2	ILE A		35.447	79.428	10.616		41.99
	ATOM	1188	CD1	ILE A	176	34.176	77.911	12.856		44.03
	ATOM	1189	N	GLU A	177	38.903	80.248	11.779	1.00	43.02
	ATOM	1190	CA	GLU A		40.162	80.444	11.058	1.00	
15	ATOM	1191	C	GLU A		41.207	80.777	12.077		44.83
13						40.907	81.329	13.126		44.24
	ATOM	1192	0	GLU A						
	ATOM	1193	CB	GLU A		40.093	81.584	10.034		44.25
	ATOM	1194	CG	GLU A		38.809	81.638	9.220		45.05
	ATOM	1195	CD	GLU A	177	38.777	80.622	8.097	1.00	46.72
20	ATOM	1196	OE1	GLU A	177	39.841	80.068	7.766	1.00	45.39
	ATOM	1197	OE2	GLU A	177	37.682	80.403	7.527	1.00	50.48
	ATOM	1198	N	PRO A		42.439	80.415	11.779		46.19
		1199		PRO A		43.546	80.666	12.688		46.98
	ATOM		CA							
	MOTA	1200	Ç	PRO A		43.634	82.100	13.117		47.64
25	ATOM	1201	0	PRO A		43.873	82.382	14.290		46.95
	ATOM	1202	CB	PRO A	178	44.761	80.306	11.853		47.61
	MOTA	1203	CG	PRO A	178	44.262	79.292	10.878	1.00	47.37
	ATOM	1204	CD	PRO A	178	42.851	79.669	10.584	1.00	46.06
	ATOM	1205	N	ASN A		43.427	83.017	12.192		48.67
30	ATOM	1206	CA	ASN A		43.621	84.414	12.547		49.57
50								13.136		49.92
	ATOM	1207	C	ASN A		42.397	85.113			
	ATOM	1208	0	ASN A		42.503	86.263	13.570	1.00	
	ATOM	1209	CB	ASN A	179	44.189	85.212	11.373	1.00	
	ATOM	1210	CG	ASN A	179	43.192	85.421	10.273		49.77
35	ATOM	1211	OD1	ASN A	179	42.186	84.732	10.192	1.00	52.40
	ATOM	1212	ND2	ASN A	179	43.486	86.357	9.396	1.00	48.53
	ATOM	1213	N	LEU A		41.267	84.418	13.215		49.23
	ATOM	1214	CA	LEU A		40.068	85.051	13.723		49.12
	ATOM	1215		LEU A		39.768	84.741	15.198		48.35
40			C							
40	ATOM	1216	0_	LEU A		40.331	83.815	15.793		47.93
	ATOM	1217	CB	LEU A		38.862	84.710	12.835		49.65
	ATOM	1218	CG	LEU A	180	38.666	85.582	11.567		52.26
	ATOM	1219	CD1	LEU A	180	39.327	86.967	11.695	1.00	53.45
	ATOM	1220	CD2	LEU A	180	39.209	84.918	10.337	1.00	53.15
45	ATOM	1221	N	PRO A		38.915	85.573	15.786	1.00	46.86
	ATOM	1222	CA	PRO A		38.511	85.431	17.179		46.36
	MOTA	1223	C	PRO A		37.861	84.100	17.474		45.21
	_					37.065	83.622	16.702		46.04
	MOTA	1224	0	PRO A	101					
	MOTA	1225	CB	PRO A		37.489	86.571	17.369		46.24
50	ATOM	1226	CG	PRO A		37.866	87.586	16.359		46.31
	ATOM	1227	CD	PRO A		38.346	86.785	15.176		47.26
	ATOM	1228	N	SER A	182	38.194	83.526	18.612	1.00	43.72
	ATOM	1229	CA	SER A		37.631	82.264	19.011	1.00	43.04
	MOTA	1230	C	SER A		36.232	82.468	19.605	1.00	42.27
55	ATOM	1231	ŏ	SER A		35.922	83.501	20.169		41.67
55						38.561	81.612	20.025		42.97
	MOTA	1232	CB	SER A						
	MOTA	1233	OG	SER A		38.449	82.245	21.280		42.30
	MOTA	1234	N	TYR A		35.369	81.490	19.424		41.67
	ATOM	1235	CA	TYR A	183	34.052	81.535	20.009		41.15
60	ATOM	1236	С	TYR A	183	34.135	80.676	21.271	1.00	39.87
	MOTA	1237	Ö	TYR A		34.633	79.553	21.207		39.01
	ATOM	1238	СB	TYR A		33.021	80.925	19.061		41.56
				TYR A		32.862	81.629	17.726		44.63
	ATOM	1239	CG							
~~	ATOM	1240	CD1	TYR A		33.729	81.369	16.672		46.43
65	MOTA	1241	CD2	TYR A		31.825	82.533	17.509		46.16
	MOTA	1242	CE1	TYR A		33.571	81.989	15.454	1.00	48.20
	MOTA	1243	CE2	TYR A	183	31.674	83.177	16.290	1.00	46.24
	ATOM	1244	CZ	TYR A	183	32.544	82.906	15.271	1.00	48.83
	ATOM	1245	OH	TYR A		32.391	83.530	14.042		51.62
70	ATOM	1246	N	ARG A		33.620	81.195	22.391		38.83
	011									

5	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1247 1248 1249 1250 1251 1252 1253	C O CB CG CD NE	ARG ARG ARG ARG ARG	A 184 A 184 A 184 A 184 A 184 A 184	33.636 32.479 31.350 33.544 33.626 34.091	79.526 79.911 81.535 80.933 81.882 81.241	23.737 23.575 24.816 26.220 27.312 28.625	1.00 36.66 1.00 36.62 1.00 38.30 1.00 39.20 1.00 38.92 1.00 39.00
10	ATOM ATOM ATOM ATOM	1255 1256 1257 1258	CZ NH1 NH2 N CA	ARG ARG A	A 184 A 185 A 185	34.541 35.125 34.460 32.745 31.674	82.966 81.096 78.250	29.759 29.768 30.891 23.968 23.984	1.00 40.63 1.00 40.89 1.00 38.62 1.00 35.61 1.00 35.15
15	ATOM ATOM ATOM ATOM	1259 1260 1261 1262 1263	C O CB CG1 CG2	ILE A ILE A ILE A	185	31.088 29.907 32.182 32.793 31.064	76.689 75.952 76.150 74.939	25.377 25.530 23.416 22.038 23.372	1.00 35.45 1.00 35.36 1.00 34.42 1.00 35.36 1.00 33.33
20	ATOM ATOM ATOM ATOM ATOM	1264 1265 1266 1267 1268	CD1 N CA C	THR ATHR ATHR A	A 186 A 186 A 186	31.872 31.923 31.481 31.870 32.751	77.091 76.745	20.993 26.393 27.742 28.715 28.448	1.00 33.99 1.00 36.11 1.00 36.38 1.00 36.91 1.00 36.47
25	ATOM ATOM ATOM ATOM ATOM	1269 1270 1271 1272 1273	CB OG1 CG2 N CA	THR ATHR ATHR ATRP ATRP	186 186 187	32.021 33.453 31.666 31.192 31.405	75.344 75.330 74.261 77.852 78.906	28.211 28.284 27.218 29.843	1.00 36.38 1.00 33.71 1.00 37.13 1.00 37.99
30	ATOM ATOM ATOM ATOM ATOM	1274 1275 1276 1277 1278	C O CB CG CD1	TRP A	187 187 187 187	31.515 31.762 30.245 30.143 29.603	78.390 79.160 79.910 80.591 80.068	30.820 32.228 33.139 30.766 29.426 28.266	1.00 39.81 1.00 39.36 1.00 40.25 1.00 40.15 1.00 43.68
35	ATOM ATOM ATOM ATOM	1279 1280 1281 1282	CD2 NE1 CE2 CE3	TRP ATRP ATRP A	187 187 187 187	30.637 29.711 30.339 31.283	81.892 80.986 82.110 82.908	29.082 27.249 27.720 29.795	1.00 44.15 1.00 45.22 1.00 44.94 1.00 43.72 1.00 47.78
40	ATOM ATOM ATOM ATOM ATOM ATOM	1283 1284 1285 1286 1287 1288	CZ2 CZ3 CH2 N CA	TRP A TRP A TRP A THR A THR A THR A	187 187 188 188	30.657 31.607 31.287 31.373 31.350 32.706	83.294 84.092 84.270 77.090 76.462	27.062 29.132 27.772 32.390 33.684	1.00 45.92 1.00 48.57 1.00 47.33 1.00 38.68 1.00 38.37
45	ATOM ATOM ATOM ATOM ATOM	1289 1290 1291 1292 1293	O CB OG1 CG2	THR A	188 188 188 188	32.833 30.458 30.904 29.049	75.969 75.440 75.251 74.443 75.667	34.141 35.246 33.568 32.463 33.224	1.00 38.26 1.00 38.27 1.00 38.31 1.00 37.24 1.00 37.94
50	ATOM ATOM ATOM ATOM ATOM	1294 1295 1296 1297 1298	N CA C O N CA	GLY A GLY A GLY A LYS A LYS A	189 189 189 190	33.710 35.023 35.476 35.295 36.074 36.541	76.093 75.565 76.074 77.246 75.209 75.583	33.283 33.606 34.957 35.247 35.769 37.117	1.00 37.93 1.00 38.12 1.00 38.04 1.00 38.63 1.00 37.97
55	ATOM ATOM ATOM ATOM ATOM	1299 1300 1301 1302 1303	C O CB CG	LYS A LYS A LYS A LYS A LYS A	190 190 190 190	37.629 37.393 35.346 35.670 34.366	74.604 73.398 75.597 76.047	37.567 37.717 38.124 39.594	1.00 38.44 1.00 37.55 1.00 36.54 1.00 38.40 1.00 41.68
60	ATOM ATOM ATOM ATOM	1304 1305 1306 1307	CE NZ N CA	LYS A LYS A GLU A GLU A	190 190 191 191	34.678 33.447 38.822 39.978	76.151 76.437 76.400 75.135 74.324	40.490 41.984 42.888 37.792 38.182	1.00 44.07 1.00 45.90 1.00 44.46 1.00 37.97 1.00 37.95
65	ATOM ATOM ATOM ATOM ATOM ATOM	1308 1309 1310 1311 1312 1313	O CB CG CD	GLU A GLU A GLU A GLU A GLU A	191 191 191 191	39.641 38.993 41.127 42.497 43.628 43.375	73.268 73.560 75.210 74.512 75.383 76.562	39.232 40.232 38.673 38.619 39.148 39.474	1.00 36.73 1.00 35.27 1.00 39.08 1.00 42.11 1.00 45.78 1.00 49.77
70	ATOM ATOM ATOM	1314 1315 1316	OE2	GLU A ASP A ASP A	191 192	44.760 40.082 39.835	74.886 72.036 70.903	39.259 38.977 39.875	1.00 47.21 1.00 35.55 1.00 35.43

	ATOM	1317	С	ASP A	192	38.394	70.518	40.097	1.00 34.50
								40.892	1.00 34.30
	ATOM	1318	0_	ASP A		38.127	69.640		
	ATOM	1319	CB		192	40.419	71.185	41.264	1.00 36.28
	ATOM	1320	CG	ASP A	192	41.923	71.224	41.257	1.00 37.00
5	ATOM	1321	OD1	ASP A	192	42.539	70.535	40.429	1.00 38.57
	ATOM	1322	OD2	ASP A	192	42.571	71.911	42.061	1.00 41.87
	ATOM	1323	N		193	37.448	71.130	39.395	1.00 33.93
	ATOM	1324	CA	ILE A		36.062	70.880	39.718	1.00 32.73
	ATOM	1325	С	ILE A		35.184	70.612	38.491	1.00 31.43
10	ATOM	1326	0	ILE A	193	34.494	69.605	38.441	1.00 30.34
	ATOM	1327	CB	ILE A	193	35.573	72.043	40.593	1.00 33.45
	ATOM	1328	CG1	ILE A		36.150	71.878	42.019	1.00 36.91
	ATOM	1329	CG2	ILE A		34.056	72.077	40.686	1.00 34.61
	ATOM	1330	CD1			36.455	73.166	42.759	1.00 40.22
15	ATOM	1331	N	ILE A	194	35.200	71.523	37.527	1.00 30.62
	ATOM	1332	CA	ILE A	194	34.448	71.376	36.312	1.00 30.28
	ATOM	1333	С	ILE A	194	35.435	71.323	35.166	1.00 29.31
	ATOM	1334	ō	ILE A		36.236	72.244	34.974	1.00 28.40
		1335		ILE A		33.446	72.525	36.102	1.00 30.93
	ATOM		CB						
20	ATOM	1336	CG1			32.462	72.643	37.267	1.00 31.11
	ATOM	1337	CG2	ILE A		32.662	72.281	34.828	1.00 32.14
	ATOM	1338	CD1	ILE A	194	31.795	71.369	37.640	1.00 32.16
	ATOM	1339	N	TYR A		35.408	70.210	34.443	1.00 28.47
	ATOM	1340	CA	TYR A		36.295	70.025	33.314	1.00 28.34
25	ATOM	1341	C	TYR A		35.475	69.894	32.017	1.00 27.52
23									
	ATOM	1342	0	TYR A		34.711	68.952	31.840	1.00 27.00
	ATOM	1343	CB	TYR A		37.147	68.746	33.481	1.00 28.77
	ATOM	1344	CG	TYR A	195	37.973	68.569	34.730	1.00 28.86
	ATOM	1345	CD1	TYR A	195	37.375	68.485	35.982	1.00 31.13
30	ATOM	1346	CD2	TYR A		39.368	68.408	34.650	1.00 29.50
50	ATOM	1347	CE1	TYR A		38.138	68.291	37.125	1.00 30.70
	ATOM	1348	CE2	TYR A		40.136	68.210	35.773	1.00 28.60
	MOTA	1349	CZ	TYR A		39.515	68.141	37.014	1.00 31.43
	ATOM	1350	OH	TYR A	195	40.250	67.942	38.161	1.00 30.49
35	ATOM	1351	N	ASN A	196	35.638	70.841	31.124	1.00 26.73
	ATOM	1352	CA	ASN A		34.971	70.787	29.832	1.00 27.22
	ATOM	1353	C	ASN A		35.995	70.465	28.744	1.00 26.56
	ATOM	1354	0	ASN A		36.911	71.241	28.528	1.00 26.95
	ATOM	1355	CB	ASN A		34.270	72.110	29.517	1.00 26.46
40	ATOM	1356	CG	ASN A	196	33.210	72.479	30.560	1.00 27.41
	ATOM	1357	OD1	ASN A	196	32.132	71.847	30.661	1.00 26.50
	ATOM	1358		ASN A		33.503	73.528	31.334	1.00 26.57
	ATOM	1359	N	GLY A		35.866	69.292	28.134	1.00 25.76
									1.00 25.70
	MOTA	1360	CA	GLY A		36.693	68.911	27.014	
45	ATOM	1361	С	GLY A		38.060	68.332	27.353	1.00 25.60
	ATOM	1362	0	GLY A	. 197	38.854	68.199	26.466	1.00 26.73
	ATOM	1363	N	ILE A	198	38.303	68.025	28.617	1.00 25.23
	ATOM	1364	CA	ILE A	198	39.517	67.405	29.102	1.00 25.68
	ATOM	1365	C	ILE A		39.075	66.541	30.259	1.00 25.94
50	ATOM	1366	_	ILE A		38.012	66.777	30.826	1.00 26.05
50			0						
	MOTA	1367	CB	ILE A		40.579	68.431	29.589	1.00 25.47
	MOTA	1368	CG1	ILE A		39.939	69.442	30.542	1.00 26.41
	ATOM	1369	CG2	ILE A	198	41.225	69.120	28.403	1.00 26.50
	ATOM	1370	CD1	ILE A	198	40.929	70.437	31.147	1.00 27.59
55	ATOM	1371	N	THR A		39.877	65.535	30.588	1.00 25.78
55				THR A		39.521	64.555	31.581	1.00 27.13
	ATOM	1372	CA						
	ATOM	1373	С	THR A		40.044	64.987	32.949	1.00 27.58
	MOTA	1374	0	THR A	199	40.994	65.765	33.006	1.00 27.38
	MOTA	1375	CB	THR A	199	40.183	63.217	31.240	1.00 27.56
60	ATOM	1376		THR A		41.546	63.434	30.778	1.00 28.44
-	MOTA	1377	CG2	THR A		39.459	62.527	30.071	1.00 29.85
	ATOM	1378	N	ASP A		39.407	64.484	34.018	1.00 27.06
	MOTA	1379	CA	ASP A		39.938	64.629	35.380	1.00 27.25
	MOTA	1380	С	ASP A		41.008	63.560	35.484	1.00 26.77
65	MOTA	1381	0	ASP A	200	41.346	62.942	34.447	1.00 26.51
	ATOM	1382	СB	ASP A		38.850	64.530	36.456	1.00 27.28
	ATOM	1383	CG	ASP A		38.352	63.124	36.651	1.00 28.95
	ATOM	1384		ASP A		38.616	62.275	35.776	1.00 25.86
	MOTA	1385		ASP A		37.708	62.761	37.671	1.00 30.54
70	MOTA	1386	N	TRP A	201	41.602	63.378	36.672	1.00 25.97

·	ATOM ATOM ATOM ATOM ATOM ATOM	1388 1389 1390 1391	3 C TRP A 20 9 O TRP A 20 10 CB TRP A 20 11 CG TRP A 20 12 CD1 TRP A 20	1 42.321 1 43.038 1 43.338 1 44.643 1 45.897	60.967 60.323 62.481 61.680 62.179	36.477 35.690 38.241 38.351 38.282	1.00 23.95 1.00 22.08 1.00 25.55 1.00 23.04 1.00 22.01
10	ATOM ATOM ATOM ATOM ATOM	1394 1395 1396 1397 1398	NE1 TRP A 20 CE2 TRP A 20 CE3 TRP A 20 CZ2 TRP A 20 CZ3 TRP A 20	1 46.815 1 46.156 1 43.903 1 46.652 1 44.394	61.169 59.978 59.201 58.694 57.931	38.521 38.406 38.550 38.644 38.682 38.773	1.00 22.38 1.00 21.58 1.00 18.42 1.00 21.85 1.00 20.23
15	ATOM ATOM ATOM ATOM ATOM ATOM	1399 1400 1401 1402 1403 1404	N VAL A 20 CA VAL A 20 C VAL A 20 O VAL A 20	2 41.199 2 40.846 2 40.493 2 40.935	57.684 60.470 59.096 58.884 57.922	38.804 37.007 36.752 35.292 34.740	1.00 22.84 1.00 23.88 1.00 22.91 1.00 21.58
20	ATOM	1404 1405 1406 1407 1408	CB VAL A 20 CG1 VAL A 20 CG2 VAL A 20 N TYR A 20 CA TYR A 20	2 39.939 2 38.597 3 39.660	58.483 57.345 59.452 59.750 59.635	37.380 38.239 37.914 34.724 33.314	1.00 24.76 1.00 24.92 1.00 27.11 1.00 23.45
25	ATOM ATOM ATOM ATOM ATOM	1409 1410 1411 1412	C TYR A 20 O TYR A 20 CB TYR A 20 CG TYR A 20	3 40.576 3 40.685 3 38.224 3 36.791	59.737 59.075 60.637 60.101	32.420 31.390 32.910 33.028	1.00 23.95 1.00 24.22 1.00 24.25 1.00 23.86 1.00 23.56
30	ATOM ATOM ATOM ATOM ATOM	1413 1414 1415 1416 1417	CD1 TYR A 20 CD2 TYR A 20 CE1 TYR A 20 CE2 TYR A 20 CZ TYR A 20	36.170 34.766 34.920 34.204	60.218 59.507 59.732 58.983 59.133	34.209 31.949 34.277 32.035 33.173	1.00 23.85 1.00 24.49 1.00 23.23 1.00 23.15 1.00 23.57
35	ATOM ATOM ATOM ATOM	1418 1419 1420 1421 1422	OH TYR A 200 N GLU A 204 CA GLU A 204 C GLU A 204 O GLU A 204	41.539 42.739 43.529 43.912	58.637 60.563 60.661 59.364 58.812	33.204 32.811 31.999 32.029 30.990	1.00 25.76 1.00 23.96 1.00 24.49 1.00 24.38 1.00 25.04
40	ATOM ATOM ATOM ATOM ATOM	1423 1424 1425 1426 1427	CB GLU A 204 CG GLU A 204 CD GLU A 204 OE1 GLU A 204 OE2 GLU A 204	45.068 46.009 45.541	61.760 61.577 62.723 63.726 62.611	32.468 31.867 32.142 32.686 31.846	1.00 24.31 1.00 25.99 1.00 23.67 1.00 28.19 1.00 22.68
45	ATOM ATOM ATOM ATOM ATOM ATOM	1428 1429 1430 1431 1432 1433	N GLU A 205 CA GLU A 205 C GLU A 205 O GLU A 205 CB GLU A 205	43.745 44.647 44.075 44.758 45.109	58.868 57.750 56.390 55.558 57.783	33.230 33.433 33.112 32.545 34.873	1.00 23.35 1.00 23.85 1.00 24.27 1.00 24.01 1.00 22.48
50	ATOM ATOM ATOM ATOM ATOM	1434 1435 1436 1437 1438	CG GLU A 205 CD GLU A 205 OE1 GLU A 205 OE2 GLU A 205 N GLU A 206 CA GLU A 206	47.329 47.716 47.903 42.826	56.779 56.653 57.564 55.581 56.182	33.565 34.421 33.504	1.00 24.17 1.00 24.44 1.00 24.45 1.00 24.40 1.00 25.05
55	ATOM ATOM ATOM ATOM ATOM	1439 1440 1441 1442 1443	C GLU A 206 O GLU A 206 CB GLU A 206 CG GLU A 206	42.214 41.080 40.927 41.673 42.711	54.889 54.703 53.599 54.606 54.739	33.502 32.512 32.018 34.908 36.005	1.00 25.30 1.00 26.38 1.00 26.34 1.00 25.85 1.00 25.12
60	ATOM ATOM ATOM ATOM	1444 1445 1446 1447	OE1 GLU A 206 OE2 GLU A 206 N VAL A 207 CA VAL A 207	43.655 43.635 44.383 40.295 39.156	53.554 52.718 53.434 55.742 55.525	36.079 35.154 37.097 32.212 31.332	1.00 26.60 1.00 24.07 1.00 23.28 1.00 26.89 1.00 26.90
65	ATOM ATOM ATOM ATOM ATOM ATOM	1448 1449 1450 1451 1452 1453	C VAL A 207 O VAL A 207 CB VAL A 207 CG1 VAL A 207 CG2 VAL A 207 N PHE A 208	39.452 39.335 37.865 36.726 37.584	55.829 54.939 56.185 55.634 55.880	29.884 29.084 31.789 30.999 33.255	1.00 27.08 1.00 27.79 1.00 27.63 1.00 24.75 1.00 26.16
70	ATOM ATOM ATOM	1454 1455 1456	CA PHE A 208 C PHE A 208 O PHE A 208	39.868 40.180 41.655 41.964	57.189	29.552 28.168 27.784 26.599	1.00 26.16 1.00 25.94 1.00 25.74 1.00 25.57

	MOTA	1457	СВ	PHE A 2	208	39.887	58.846	27.841	1.00	25.16
	ATOM	1458	CG	PHE A 2		38.453	59.246	27.884		25.82
	ATOM	1459		PHE A 2		37.441	58.346	28.011		28.40
			-							
_	MOTA	1460	-	PHE A 2		38.126	60.587	27.774		28.74
5	ATOM	1461	CE1			36.138	58.765	28.026	1.00	
	ATOM	1462	CE2			36.841	61.009	27.809		27.47
	MOTA	1463	cz	PHE A 2		35.842	60.088	27.918		28.83
	MOTA	1464	N	SER A 2	209	42.562	57.097	28.755	1.00	25.92
	ATOM	1465	CA	SER A 2	209	44.025	57.083	28.461	1.00	26.32
10	ATOM	1466	C	SER A 2		44.408	58.267	27.598	1.00	
	ATOM	1467	ŏ	SER A 2		45.199	58.162	26.634		25.56
	ATOM	1468	СВ	SER A 2		44.491	55.779	27.788		26.23
	ATOM	1469	OG	SER A 2		44.260	54.669	28.654		28.15
	ATOM	1470	N	ALA A 2		43.873	59.415	27.964		25.14
15	MOTA	1471	CA	ALA A 2		44.112	60.612	27.206		25.32
	MOTA	1472	С	ALA A 2	210	43.541	61.773	27.956	1.00	24.94
	MOTA	1473	0	ALA A 2	210	42.607	61.602	28.749	1.00	25.25
	ATOM	1474	CB	ALA A 2	210	43.427	60.472	25.805	1.00	26.30
	ATOM	1475	N	TYR A 2		44.117	62.945	27.746		25.21
20	ATOM	1476	CA	TYR A 2		43.635	64.183	28.341		25.71
20	ATOM	1477	C	TYR A 2		42.431	64.718	27.600		26.13
	MOTA	1478	0	TYR A 2		41.541	65.335	28.189		27.81
	MOTA	1479	CB	TYR A 2		44.709	65.241	28.293		25.39
	MOTA	1480	CG	TYR A 2	11	44.486	66.458	29.201		26.84
25	MOTA	1481	CD1	TYR A 2	11	43.726	66.388	30.368	1.00	28.16
	ATOM	1482	CD2	TYR A 2	11	45.103	67.649	28.912	1.00	28.94
	ATOM	1483	CE1	TYR A 2	11	43.580	67.503	31.206	1.00	27.97
	ATOM	1484	CE2	TYR A 2	11	44.986	68.738	29.736		31.54
	ATOM	1485	CZ	TYR A 2		44.217	68.653	30.892		29.76
30	ATOM	1486	OH	TYR A 2		44.094	69.774	31.654		28.46
50		1487								
	ATOM		N	SER A 2		42.393	64.494	26.297		26.81
	MOTA	1488	CA	SER A 2		41.339	65.067	25.490		26.75
	ATOM	1489	С	SER A 2		39.978	64.470	25.719		26.28
	ATOM	1490	0	SER A 2	12	39.837	63.264	25.890		24.94
35	ATOM	1491	CB	SER A 2	12	41.627	64.896	24.022	1.00	27.36
	ATOM	1492	OG	SER A 2	12	40.665	65.666	23.334	1.00	30.68
	ATOM	1493	N	ALA A 2		38.966	65.333	25.717		26.33
	ATOM	1494	CA	ALA A 2		37.614	64.864	25.821		26.95
	ATOM	1495	C	ALA A 2		36.758	65.656	24.847		27.47
40	ATOM	1496								
40			0	ALA A 2		35.665	66.116	25.190		26.21
	ATOM	1497	CB	ALA A 2		37.119	65.001	27.240		28.10
	ATOM	1498	N	LEU A 2		37.297	65.781	23.628		27.83
	ATOM	1499	CA	LEU A 2		36.675	66.459	22.488		28.52
	ATOM	1500	С	LEU A 2	14	36.680	65.512	21.249	1.00	28.36
45	ATOM	1501	0	LEU A 2	14	37.685	64.886	20.948	1.00	26.65
	MOTA	1502	CB	LEU A 2	14	37.477	67.719	22.104	1.00	29.14
	ATOM	1503	CG	LEU A 2		37.670	68.866	23.103		30.74
	ATOM	1504		LEU A 2		38.515	69.912	22.501		32.71
		1505		LEU A 2		36.363	69.457	23.442		
50	ATOM ATOM									31.48
50		1506	N	TRP A 2		35.581	65.472	20.504		28.74
	MOTA	1507	CA	TRP A 2		35.499	64.653	19.296		29.38
	ATOM	1508	С	TRP A 2		34.829	65.419	18.180		29.51
	ATOM	1509	0	TRP A 2	15	33.624	65.644	18.208	1.00	28.64
	ATOM	1510	CB	TRP A 2	15	34.719	63.378	19.571	1.00	28.75
55	ATOM	1511	CG	TRP A 2		35.313	62.597	20.678		28.51
	ATOM	1512		TRP A 2		36.238	61.608	20.582		29.30
	ATOM	1513		TRP A 2		35.053	62.765	22.084		30.05
		1514		TRP A 2		36.555	61.125	21.841		27.30
	ATOM									
C C	ATOM	1515		TRP A 2		35.844	61.818	22.778		28.78
60	MOTA	1516				34.225	63.612	22.824		29.11
	ATOM	1517				35.825	61.692	24.165		27.86
	ATOM	1518	CZ3	TRP A 2	15	34.204	63.486	24.192	1.00	29.94
	ATOM	1519		TRP A 2	15	35.003	62.521	24.852		29.39
	ATOM	1520	N	TRP A 2		35.624	65.867	17.224		30.56
65	ATOM	1521	CA	TRP A 2		35.084	66.533	16.037		31.55
	ATOM	1522	C	TRP A 2		34.417	65.488	15.143		32.02
	ATOM		0	TRP A 2		34.866				
		1523					64.370	15.089		31.09
	ATOM	1524	CB	TRP A 2		36.202	67.133	15.221		32.03
	ATOM	1525	CG	TRP A 2		36.828	68.453	15.659		32.53
70	ATOM	1526	CD1	TRP A 2	16	38.047	68.623	16.234	1.00	35.04

	5		1527 1528 1529 1530 1531	NE CE CE CZ	1 TRP A 216 2 TRP A 216 3 TRP A 216 2 TRP A 216	36.318 38.318 37.259 35.146 37.076	69.957	15.428 16.399 15.924 14.868 15.866	1.00 35.73 1.00 34.58 1.00 33.81
	10	ATOM ATOM ATOM ATOM ATOM ATOM	1532 1533 1534 1535 1536 1537	CH: N CA C	2 TRP A 216 SER A 217 SER A 217 SER A 217 SER A 217	34.967 35.930 33.331 32.698 33.629 34.552	71.608 72.491 65.853 64.963 64.910 65.709	14.811 15.310 14.455 13.494 12.267 12.145	1.00 35.33 1.00 33.12 1.00 33.26
	15	ATOM ATOM ATOM ATOM ATOM ATOM	1538 1539 1540 1541 1542 1543	og N	SER A 217 SER A 217 PRO A 218 PRO A 218 PRO A 218 PRO A 218	31.289 31.362 33.463 34.421 34.404 35.442	65.465 66.694 63.936 63.810 65.047 65.464	13.119 12.380 11.381 10.260 9.348 8.877	1.00 33.02 1.00 33.81 1.00 34.85 1.00 35.78 1.00 36.49 1.00 36.64
	20	ATOM ATOM ATOM ATOM ATOM	1544 1545 1546 1547 1548	CB CG CD N CA	PRO A 218 PRO A 218 PRO A 218 ASN A 219 ASN A 219	34.005 33.048 32.423 33.236 33.011	62.513 61.787 62.899 65.634 66.915	9.563 10.573 11.388 9.177	1.00 36.92 1.00 35.44 1.00 34.89 1.00 37.94
ļ	25	ATOM ATOM ATOM ATOM ATOM	1549 1550 1551 1552 1553	C O CB CG	ASN A 219 ASN A 219 ASN A 219 ASN A 219 ASN A 219	33.683 33.913 31.519 30.787	68.167 69.187 67.268 67.317	8.483 9.086 8.395 8.647 7.360	1.00 39.83 1.00 40.56 1.00 40.45 1.00 39.50 1.00 41.31
	30	ATOM ATOM ATOM ATOM	1554 1555 1556 1557	ND2 N CA C	GLY A 220 GLY A 220 GLY A 220 GLY A 220	31.380 29.472 33.869 34.267 33.044	67.108 67.605 68.125 69.296 70.160	6.320 7.409 10.404 11.139 11.406	1.00 46.10 1.00 39.61 1.00 40.09 1.00 40.36 1.00 40.26
	35	ATOM ATOM ATOM ATOM ATOM	1558 1559 1560 1561 1562	O N CA C	GLY A 220 THR A 221 THR A 221 THR A 221 THR A 221	33.157 31.865 30.644 30.442 30.412	71.298 69.607 70.340 70.461 71.573	11.808 11.192 11.402 12.899 13.433	1.00 40.94 1.00 40.25 1.00 40.02 1.00 39.77 1.00 39.48
	40	ATOM ATOM ATOM ATOM ATOM	1563 1564 1565 1566 1567	CB OG1 CG2 N CA		29.493 29.619 28.189 30.337 30.094	69.574 69.594 70.258 69.292 69.165	10.772 9.347 10.991 13.548 14.965	1.00 40.24 1.00 42.51 1.00 42.08 1.00 38.47 1.00 37.43
	45	ATOM ATOM ATOM ATOM ATOM	1568 1569 1570 1571 1572	C O CB CG CD1	PHE A 222 PHE A 222 PHE A 222 PHE A 222 PHE A 222	31.312 32.184 29.177 27.878 26.830	68.859 68.058 67.985 68.040 68.768	15.815 15.411 15.216 14.490 14.996	1.00 37.43 1.00 36.12 1.00 35.24 1.00 37.84 1.00 39.38 1.00 39.66
	50	ATOM ATOM ATOM ATOM ATOM	1573 1574 1575 1576 1577	CD2 CE1 CE2 CZ N	PHE A 222 PHE A 222 PHE A 222 PHE A 222 LEU A 223	27.693 25.605 26.488 25.435 31.297	67.310 68.804 67.332 68.078 69.458	13.320 14.331 12.661 13.168 17.015	1.00 39.54 1.00 41.91 1.00 40.33 1.00 40.84 1.00 34.08
	55	ATOM ATOM ATOM ATOM ATOM ATOM	1578 1579 1580 1581 1582	CA C O CB CG	LEU A 223 LEU A 223 LEU A 223 LEU A 223 LEU A 223	32.253 31.474 30.575 32.814 34.272	69.207 68.612 69.264 70.487 70.592	18.093 19.231 19.804 18.622 19.033	1.00 32.28 1.00 31.26 1.00 30.76 1.00 31.83 1.00 31.24
	60	ATOM ATOM ATOM ATOM	1583 1584 1585 1586 1587	CD2 N CA C	LEU A 223 LEU A 223 ALA A 224 ALA A 224 ALA A 224	34.305 35.040 31.780 31.167 32.211	71.384 69.292 67.373 66.759 66.839	20.261 19.185 19.546 20.667 21.766	1.00 27.64 1.00 30.20 1.00 29.71 1.00 29.39 1.00 29.58
	65	ATOM ATOM ATOM ATOM ATOM	1588 1589 1590 1591 1592	O CB N CA C	ALA A 224 ALA A 224 TYR A 225 TYR A 225 TYR A 225	33.414 30.815 31.746 32.624 31.951	66.879 65.374 66.905 66.979 66.480	21.481 20.381 23.004 24.160 25.451	1.00 29.87 1.00 29.73 1.00 28.33 1.00 28.44 1.00 27.99
	70	ATOM ATOM ATOM ATOM	1593 1594 1595 1596	O CB CG CD1	TYR A 225 TYR A 225 TYR A 225 TYR A 225	30.705 33.106 32.029 31.692	66.397 68.386 69.376 69.521	25.551 24.375 24.813 26.145	1.00 27.26 1.00 28.46 1.00 32.08 1.00 32.98

	ATOM ATOM	1597 1598	CD2	TYR A	225	31.395 30.742	70.201 70.421	23.894 26.541	1.00	35.25 35.61
	ATOM ATOM	1599 1600	CE2	TYR A		30.453 30.125	71.137 71.227	24.295 25.616	1.00	35.83 36.19
5	ATOM	1601	OH	TYR A		29.195	72.133	26.040	1.00	
	MOTA	1602	N	ALA A		32.806	66.130	26.415	1.00	
	ATOM	1603	CA	ALA A		32.399	65.607	27.689	1.00	
	ATOM ATOM	1604 1605	C O	ALA A ALA A		32.764 33.718	66.611 67.428	28.743 28.572	$1.00 \\ 1.00$	
10	ATOM	1606	СВ	ALA A		33.052	64.303	27.961	1.00	
	ATOM	1607	N	GLN A	227	31.979	66.590	29.821	1.00	
	ATOM	1608	CA	GLN A		32.178	67.501	30.913	1.00	
	ATOM ATOM	1609 1610	C O	GLN A GLN A		32.153 31.233	66.680 65.922	32.133 32.313	1.00	26.18 25.02
15	ATOM	1611	СВ	GLN A		31.066	68.534	31.012	1.00	
	ATOM	1612	CG	GLN A		31.129	69.423	32.276	1.00	
	ATOM	1613	CD	GLN A		29.856	70.174	32.462		25.53
	MOTA ATOM	1614 1615	OE1 NE2			28.932 29.772	69.635 71.394	33.057 31.914		26.19 26.60
20	ATOM	1616	N	PHE A		33.187	66.846	32.948		25.69
	ATOM	1617	CA	PHE A		33.363	66.112	34.190	1.00	26.42
	ATOM	1618	C	PHE A		33.228	67.057	35.414		27.26
	ATOM ATOM	1619 1620	O CB	PHE A		33.673 34.722	68.204 65.395	35.411 34.210	1.00	27.24 25.89
25	ATOM	1621	CG	PHE A		34.957	64.479	33.015	1.00	24.46
	MOTA	1622	CD1			34.352	63.243	32.933		23.87
	ATOM	1623	CD2			35.735	64.871	31.997	1.00	23.06
	ATOM ATOM	1624 1625	CE1 CE2			34.547 35.928	62.444 64.054	31.869 30.915	1.00	23.93 25.34
30	ATOM	1626	CZ	PHE A		35.322	62.852	30.852		23.94
	ATOM	1627	N	ASN A	-	32.568	66.551	36.434		28.68
	ATOM	1628 1629	CA	ASN A		32.295	67.292	37.659	1.00	29.51
	ATOM ATOM	1630	c o	ASN A ASN A		32.904 32.467	66.514 65.417	38.786 39.049		29.69 29.16
35	ATOM	1631	ČВ	ASN A		30.781	67.371	37.879		30.11
	ATOM	1632	CG	ASN A		30.409	68.340	38.981		30.80
	ATOM ATOM	1633 1634	OD1 ND2	ASN A ASN A		31.127 29.280	68.432 69.083	39.990 38.778	1.00	27.42 30.54
	ATOM	1635	NDZ N	ASN A		33.923	67.085	39.435		31.03
40	ATOM	1636	CA	ASP A		34.614	66.413	40.525		31.69
	ATOM	1637	C	ASP A		34.302	67.071	41.890		31.33
	ATOM ATOM	1638 1639	O CB	ASP A ASP A		34.968 36.120	66.822 66.408	42.883 40.231		31.35 31.98
	ATOM	1640	CG	ASP A		36.512	65.329	39.212		33.87
45	MOTA	1641		ASP A	230	35.938	65.329	38.087		32.91
	ATOM	1642		ASP A		37.361	64.439	39.458		33.90
	ATOM ATOM	1643 1644	N CA	THR A		33.255 32.858	67.868	41.935 43.170		31.67 32.12
	ATOM	1645	Ċ.	THR A		33.045	67.790	44.458		32.06
50	MOTA	1646	0	THR A	231	33.673	68.307	45.387	1.00	32.58
	ATOM	1647	CB	THR A		31.416 31.318	69.087	43.087 42.046		32.16 31.97
	ATOM ATOM	1648 1649	OG1	THR A		31.048	70.061 69.939	44.353		34.78
	ATOM	1650	N	GLU A		32.518	66.574	44.525		31.58
55	MOTA	1651	CA	GLU A		32.633	65.782	45.746		31.96
	ATOM	1652 1653	C O	GLU A GLU A		33.679 33.591	64.684 63.772	45.675 46.436		30.11 29.23
	ATOM ATOM	1654	СВ	GLU A		31.273	65.070	46.430		33.29
	ATOM	1655	CG	GLU A		30.064	65.973	46.295		36.12
60	MOTA	1656	CD	GLU A		28.797	65.181	46.584		42.23
	ATOM	1657		GLU A		28.699	64.561	47.690		46.60
	ATOM ATOM	1658 1659	N N	GLU A VAL A		27.910 34.595	65.145 64.674	45.696 44.709		43.91 28.95
	ATOM	1660	CA	VAL A		35.585	63.588	44.698	1.00	28.12
65	ATOM	1661	C	VAL A	233	36.618	64.015	45.717	1.00	26.69
	ATOM ATOM	1662 1663	O CB	VAL A VAL A		37.020 36.300	65.149 63.426	45.677 43.333		25.94 27.51
	ATOM	1664		VAL A		37.297	62.296	43.333		27.86
	ATOM	1665		VAL A	233	35.316	63.155	42.235		29.07
70	MOTA	1666	N	PRO A	234	37.017	63.161	46.638	1.00	26.33

5	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1667 1668 1669 1670 1671 1672 1673	C O CB CG CD	PRO A 234 PRO A 234 PRO A 234 PRO A 234 PRO A 234	39.406 39.704 38.062 36.840 36.566	63.783 63.379 62.358 61.566 61.777	47.609 46.991 45.845 48.564 48.293 46.860	1.00 26.79 1.00 27.08 1.00 26.15 1.00 27.74 1.00 26.40 1.00 27.06
10	ATOM ATOM ATOM ATOM ATOM	1674 1675 1676 1677 1678	N CA C O CB CG	LEU A 235 LEU A 235 LEU A 235 LEU A 235 LEU A 235 LEU A 235	41.537 42.615 42.621	64.459 64.873 64.040 63.857 66.300 67.294	47.764 47.289 47.830 48.996 47.752 47.277	1.00 26.80 1.00 27.73 1.00 26.54 1.00 26.56 1.00 28.91 1.00 31.69
15	ATOM ATOM ATOM ATOM ATOM ATOM	1679 1680 1681 1682 1683 1684	CD1 CD2 N CA C	LEU A 235 LEU A 235 ILE A 236 ILE A 236 ILE A 236 ILE A 236	40.920 40.820 43.504 44.723 45.668 45.717	68.649 67.410 63.487 62.929 64.117	47.957 45.771 47.004 47.574 47.741	1.00 32.34 1.00 32.38 1.00 25.35 1.00 25.28 1.00 25.50
20	ATOM ATOM ATOM ATOM	1685 1686 1687 1688	CB CG1 CG2 CD1	ILE A 236 ILE A 236 ILE A 236	45.341 46.695 45.651	65.003 61.848 61.374 62.336	46.891 46.716 47.307 45.346	1.00 26.26 1.00 25.40 1.00 25.58 1.00 24.79
25	ATOM ATOM ATOM ATOM ATOM	1689 1690 1691 1692 1693	N CA C O CB	GLU A 237 GLU A 237 GLU A 237 GLU A 237 GLU A 237	46.610 46.423 47.343 48.706 48.809 46.834	60.657 64.127 65.227 64.679 63.702 66.023	48.552 48.828 49.166 49.490 50.219 50.364	1.00 24.55 1.00 25.87 1.00 26.29 1.00 26.07 1.00 26.68 1.00 25.50
30	ATOM ATOM ATOM ATOM ATOM	1694 1695 1696 1697 1698	CG CD OE1 OE2 N		45.506 45.044 45.470 44.245 49.750	66.661 67.593 67.411 68.498 65.277	50.098 51.197 52.326 50.924 48.914	1.00 28.14 1.00 30.95 1.00 36.58 1.00 33.62 1.00 25.45
35	ATOM ATOM ATOM ATOM ATOM	1699 1700 1701 1702 1703	CA C O CB CG	TYR A 238 TYR A 238 TYR A 238 TYR A 238 TYR A 238	51.112 52.014 51.636 51.563 51.416	64.861 66.056 67.011 63.678	49.221 49.002 48.319 48.371	1.00 25.12 1.00 25.07 1.00 24.71 1.00 25.28
40	ATOM ATOM ATOM ATOM ATOM	1704 1705 1706 1707 1708	CD1 CD2 CE1 CE2 CZ	TYR A 238 TYR A 238 TYR A 238 TYR A 238 TYR A 238	52.438 50.255 52.306 50.089 51.112	63.908 64.483 63.542 64.657 63.744 64.298	46.868 46.123 46.201 44.717 44.810 44.078	1.00 24.32 1.00 24.57 1.00 26.15 1.00 25.65 1.00 25.06 1.00 27.74
45	ATOM ATOM ATOM ATOM ATOM	1709 1710 1711 1712 1713	OH N CA C	TYR A 238 SER A 239 SER A 239 SER A 239 SER A 239	50.935 53.198 54.149 54.986 55.279	64.498 65.991 67.099 67.085	42.721 49.592 49.589 48.329	1.00 29.66 1.00 24.64 1.00 25.18 1.00 25.42
50	ATOM ATOM ATOM ATOM ATOM	1714 1715 1716 1717 1718	CB OG N CA C	SER A 239 SER A 239 PHE A 240 PHE A 240 PHE A 240	55.279 55.094 54.433 55.303 56.235 57.338	66.013 66.970 67.261 68.259 68.334 69.297	47.835 50.788 51.996 47.770 46.636 47.116	1.00 25.65 1.00 23.96 1.00 26.38 1.00 25.12 1.00 27.19 1.00 27.23
55	ATOM ATOM ATOM ATOM ATOM	1719 1720 1721 1722 1723		PHE A 240 PHE A 240 PHE A 240 PHE A 240 PHE A 240	57.045 55.561 56.423 56.436 57.180	70.421 68.831 68.708 67.560 69.758	47.479 45.338 44.091 43.366 43.652	1.00 28.10 1.00 27.32 1.00 26.88 1.00 29.66 1.00 26.22
60	ATOM ATOM ATOM ATOM ATOM	1724 1725 1726 1727	CE1 CE2 CZ N	PHE A 240 PHE A 240 PHE A 240 TYR A 241	57.219 57.948 57.973 58.585	67.440 69.661 68.483 68.849	42.209 42.556 41.804 47.126	1.00 31.46 1.00 29.05 1.00 30.46 1.00 27.65
65	ATOM ATOM ATOM ATOM ATOM	1728 1729 1730 1731 1732 1733	C O CB CG	TYR A 241 TYR A 241 TYR A 241 TYR A 241 TYR A 241 TYR A 241	59.682 60.310 60.774 60.713 60.043 59.699	69.646 70.677 71.706 68.702 67.793 68.266	47.733 46.794 47.236 48.345 49.350 50.584	1.00 27.45 1.00 27.41 1.00 27.31 1.00 27.05 1.00 25.67 1.00 25.88
70	ATOM ATOM ATOM	1734 1735 1736	CD2 CE1	TYR A 241 TYR A 241 TYR A 241	59.644 59.026 58.962	66.509 67.492 65.716	49.023 51.499 49.949	1.00 25.17 1.00 22.03 1.00 25.79

	ATOM	1737	CZ	TVP	Δ	241		58.653	66.227	51.190	1 00	23.56
						241						
	MOTA	1738	ОН					57.963	65.495	52.149	1.00	
	ATOM	1739	N	SER	Α	242		60.253	70.413	45.497	1.00	27.48
	ATOM	1740	CA	SER	Α	242		60.798	71.303	44.478	1 00	28.37
5		1741				242		62.315	71.519	44.630		28.05
3	MOTA		C									
	ATOM	1742	0			242		62.977	70.770	45.298	1.00	25.76
	ATOM	1743	CB	SER	Α	242		60.059	72.632	44.493	1.00	28.30
	ATOM	1744	ŌĞ			242		60.394	73.384	43.322		30.80
	ATOM	1745	N			243		62.841	72.551	43.985		29.45
10	ATOM	1746	CA	ASP	Α	243		64.239	72.889	44.103	1.00	30.35
	ATOM	1747	С	ACD	Δ	243		64.607	73.246	45.548	1.00	30.57
												29.24
	ATOM	1748	0			243		63.767	73.633	46.347		
	ATOM	1749	СВ	ASP	Α	243		64.525	74.099	43.236	1.00	31.66
	ATOM	1750	CG	ASP	Α	243		64.376	73.792	41.724	1.00	37.62
15	ATOM	1751		ASP				64.539	72.598	41.307		41.54
13												
	ATOM	1752	OD2					64.094	74.696	40.888		43.31
	ATOM	1753	N	GLU	Α	244		65.889	73.163	45.849	1.00	31.16
	ATOM	1754	CA	CLII	Α	244		66.398	73.505	47.156	1 00	32.38
		1755				244		65.909	74.835	47.691		32.53
	ATOM		Ç									
20	ATOM	1756	0	GLU	Α	244		65.763	75.013	48.916		29.71
	ATOM	1757	CB	GLU	Α	244		67.895	73.640	47.058	1.00	32.97
	ATOM	1758	CG			244		68.599	73.090	48.244	1 00	36.11
												_
	ATOM	1759	CD			244		70.079	73.349	48.175		38.61
	MOTA	1760	OE1	GLU	Α	244		70.673	72.877	47.190	1.00	37.80
25	ATOM	1761	OE2	GLU	Α	244		70.612	74.004	49.096	1.00	38.10
	ATOM	1762	N			245		65.716	75.778	46.755		32.65
	MOTA	1763	CA			245		65.358	77.145	47.080		32.39
	ATOM	1764	С	SER	Α	245		63.979	77.307	47.670	1.00	32.11
	ATOM	1765	0	SER	А	245		63.696	78.337	48.272	1 00	32.83
30	ATOM	1766	ČВ					65.490	78.040	45.846		32.75
50												
	ATOM	1767	OG			245		64.890	77.446	44.715		34.54
	ATOM	1768	N	LEU	Α	246		63.110	76.311	47.547	1.00	31.96
	ATOM	1769	CA	LEU				61.750	76.508	48.086	1 00	31.53
	MOTA	1770	C	LEU				61.838	76.325	49.579		29.60
35	ATOM	1771	0	LEU	А	246		62.186	75.250	50.040	1.00	27.72
	ATOM	1772	CB	LEU	Α	246		60.730	75.520	47.518	1.00	31.55
	ATOM	1773	CG	LEU				59.289	75.989	47.192		35.35
	MOTA	1774		LEU				58.258	74.803	47.222		36.22
	ATOM	1775	CD2	LEU	Α	246		58.759	77.136	47.970	1.00	34.37
40	ATOM	1776	N	GLN	А	247		61.493	77.376	50.319	1.00	28.90
	ATOM	1777	CA	GLN				61.577	77.346	51.762		27.73
	ATOM	1778	С	GLN				60.535	76.405	52.413		27.30
	ATOM	1779	0	GLN	Α	247		60.857	75.551	53.263	1.00	25.43
	ATOM	1780	CB	GLN	Α	247		61.510	78.759	52.314	1.00	28.64
45	ATOM	1781	CG	GLN				61.637	78.795	53.838		28.67
40												
	ATOM	1782	CD	GLN				61.930	80.174	54.399	1.00	30.01
	ATOM	1783	OE1	GLN	Α	247		62.833	80.347	55.276	1.00	28.72
	ATOM	1784	NE2	GLN	Δ	247		61.177	81.152	53.940	1 00	29 07
										00.2.0		26.79
	MOTA	1785	N	TYR				59.305	76.502	51.946		
50	ATOM	1786	CA	TYR				58.231	75.642	52.422		26.56
	ATOM	1787	С	TYR	Α	248		57.767	74.732	51.288	1.00	26.50
	ATOM	1788	Ō	TYR				57.536	75.189	50.161		26.57
	ATOM	1789	СВ	TYR				57.029	76.433	52.838		26.24
	ATOM	1790	CG	TYR	Α	248		57.240	77.264	54.079	1.00	27.06
55	ATOM	1791	CD1	TYR	Α	248		57.980	78.450	54.039	1.00	26.07
-	ATOM	1792	CD2	TYR				56.685	76.875	55.285		24.74
	ATOM	1793	CE1	TYR				58.175	79.206	55.193		28.15
	ATOM	1794	CE2	TYR	Α	248		56.884	77.617	56.448	1.00	23.55
	ATOM	1795	CZ	TYR				57.605	78.774	56.410		25.61
60	ATOM	1796	OH	TYR				57.744	79.500			25.29
UU										57.583		
	ATOM	1797	N	PRO				57.664	73.457	51.583		25.69
	ATOM	1798	CA	PRO	Α	249		57.186	72.489	50.608	1.00	26.62
	ATOM	1799	C	PRO				55.756	72.782	50.169		27.20
	ATOM	1800	0	PRO				54.943	73.334	50.908		24.53
65	ATOM	1801	CB	PRO				57.238	71.166	51.373	1.00	27.47
	ATOM	1802	CG	PRO	Α	249	۵	58.249	71.400	52.431		27.65
	ATOM	1803	CD	PRO			-	58.019	72.840	52.862		25.35
									72.040			
	ATOM	1804	N	LYS				55.466	72.391	48.937		28.36
	ATOM	1805	CA	LYS	Α	250		54.179	72.636	48.335	1.00	30.14
70	ATOM	1806	C	LYS				53.342	71.406	48.673		29.50
			~					22.342		20.073		

					0.	_		
	ATOM		0	LYS A 250	53.88	3 70.327	48.852	2 1.00 31.02
	ATOM			LYS A 250	54.40	7 72.812	46.805	1.00 30.66
	ATOM ATOM			LYS A 250 LYS A 250				
	5 ATOM			LYS A 250				
	ATOM	1812		LYS A 250	52.685	73.611		1.00 45.13
	ATOM ATOM	1813 1814	N CA	THR A 251		2 71.571	48.878	1.00 29.70
	ATOM	1815	CA	THR A 251 THR A 251				
10		1816	ō	THR A 251				
	ATOM	1817	CB	THR A 251	50.135	70.660		
	ATOM ATOM	1818 1819	OG1 CG2				51.434	
	ATOM	1820	N CG2	VAL A 251			50.230 47.025	
15		1821	CA	VAL A 252	49.828		45.793	
	MOTA ATOM	1822 1823	C	VAL A 252			46.149	1.00 27.81
	ATOM	1824	O CB	VAL A 252 VAL A 252			47.002	
	ATOM	1825		VAL A 252	49.763		44.908 43.712	1.00 29.42 1.00 31.02
20		1826	CG2	VAL A 252	51.887	68.656	44.459	1.00 31.02
	ATOM ATOM	1827 1828	N CA	ARG A 253 ARG A 253	47.425	_	45.519	1.00 27.54
	ATOM	1829	C	ARG A 253	46.066 45.369		45.804 44.528	
	ATOM	1830	O	ARG A 253	45.202		43.684	1.00 26.49 1.00 26.20
25	ATOM ATOM	1831	CB	ARG A 253	45.215		46.533	1.00 29.21
	ATOM	1832 1833	CG CD	ARG A 253 ARG A 253	45.749 45.055		47.911	1.00 31.87
	MOTA	1834	NE	ARG A 253	45.528		48.487 47.756	1.00 39.81 1.00 49.04
20	ATOM	1835	CZ	ARG A 253	46.583	73.015	48.126	1.00 54.08
30	ATOM ATOM	1836 1837	NH1 NH2	ARG A 253 ARG A 253	47.260		49.254	1.00 51.93
	ATOM	1838	N	VAL A 254	46.938 44.897	74.053 66.701	47.375 44.414	1.00 56.78 1.00 26.67
	ATOM	1839	CA	VAL A 254	44.282	66.249	43.178	1.00 26.16
35	ATOM ATOM	1840 1841	C O	VAL A 254 VAL A 254	43.055	65.428	43.507	1.00 26.32
	ATOM	1842	CB	VAL A 254	43.119 45.218	64.558 65.280	44.369 42.442	1.00 25.35
	MOTA	1843		VAL A 254	44.594	64.755	41.129	1.00 27.20 1.00 26.94
	ATOM ATOM	1844 1845	CG2		46.593	65.917	42.198	1.00 27.66
40	ATOM	1845	N CA	PRO A 255 PRO A 255	41.951 40.759	65.684	42.810	1.00 24.55
	ATOM	1847	C	PRO A 255	41.057	64.856 63.482	42.931 42.339	1.00 24.42 1.00 23.94
	ATOM	1848	0	PRO A 255	41.366	63.386	41.161	1.00 24.49
	ATOM ATOM	1849 1850	CB CG	PRO A 255 PRO A 255	39.712	65.621	42.117	1.00 24.86
45	ATOM	1851	CD	PRO A 255	40.213 41.743	66.975 66.781	41.956 41.867	1.00 24.37 1.00 25.52
	ATOM	1852	N	TYR A 256	40.923	62.466	43.167	1.00 23.32
	ATOM ATOM	1853	CA	TYR A 256	41.305	61.150	42.888	1.00 21.42
	ATOM	1854 1855	С 0	TYR A 256 TYR A 256	40.424 40.562	60.239 60.188	43.690 44.896	1.00 21.84
50	MOTA	1856	CB	TYR A 256	42.725	60.968	43.414	1.00 22.15 1.00 20.43
	MOTA	1857	CG	TYR A 256	43.336	59.599	43.166	1.00 20.95
	ATOM ATOM	1858 1859		TYR A 256 TYR A 256	42.920 44.371	58.486	43.867	1.00 22.41
	ATOM	1860		TYR A 256	43.500	59.440 57.259	42.283 43.687	1.00 19.15 1.00 21.46
5 5	ATOM	1861	CE2	TYR A 256	44.948	58.223	42.083	1.00 21.40
	ATOM ATOM	1862 1863		TYR A 256	44.535	57.129	42.781	1.00 21.87
	ATOM	1864		TYR A 256 PRO A 257	45.127 39.560	55.875 59.467	42.546	1.00 19.77
	ATOM	1865		PRO A 257	38.666	58.524	43.031 43.725	1.00 22.36 1.00 22.11
60	ATOM	1866		PRO A 257	39.325	57.225	44.064	1.00 22.59
	ATOM ATOM	1867 1868		PRO A 257	39.655	56.471	43.148	1.00 24.08
	ATOM			PRO A 257 PRO A 257	37.535 38.102	58.252 58.730	42.700	1.00 22.29
	ATOM	1870		PRO A 257	39.311	59.551	41.316 41.588	1.00 23.05 1.00 22.21
65	MOTA			LYS A 258	39.487	56.926	45.340	1.00 21.64
	ATOM ATOM			LYS A 258 LYS A 258	40.003	55.658	45.750	1.00 21.77
	ATOM			LYS A 258	38.828 37.704	54.695 55.116	45.750 45.589	1.00 22.73
70	MOTA	1875	CB I	LYS A 258	40.737	55.745	47.096	1.00 22.89 1.00 21.30
70	MOTA	1876	CG 1	LYS A 258	41.902	56.717	47.043	1.00 21.60

	ATOM	1877	$^{\mathtt{CD}}$	LYS A 2	58	42.551	57.039	48.388	1.00	22.69
	ATOM	1878	CE	LYS A 2		43.967	57.664	48.222	1.00	
	ATOM	1879	ΝZ	LYS A 2		45.102	56.699	48.446	1.00	
	ATOM	1880	N	ALA A 2	59	39.111	53.404	45.849	1.00	23.38
5	ATOM	1881	CA	ALA A 2	. 0	38.100	52.365	45.759		25.01
,										
	MOTA	1882	С	ALA A 2		36.915	52.595	46.691		26.15
	ATOM	1883	0	ALA A 2	59	37.08 7	52.705	47.920	1.00	24.93
	ATOM	1884		ALA A 2		38.723	51.017	46.042	1.00	
			CB							
	ATOM	1885	N	GLY A 2	0	35.722	52.685	46.083	1.00	25.93
10	ATOM	1886	CA	GLY A 2	60	34.493	52.907	46.818	1 00	26.52
	ATOM	1887	Ç	GLY A 2		34.231	54.369	47.166	1.00	
	ATOM	1888	0	GLY A 2	50	33.297	54.671	47.868	1.00	28.17
	ATOM	1889	N	ALA A 2	1	35.031	55.301	46.681	1 00	27.63
	ATOM	1890	CA	ALA A 2		34.779	56.694	47.042		27.82
15	ATOM	1891	С	ALA A 2	51	33.853	57.342	46.022	1.00	27.48
	ATOM	1892	0	ALA A 2		33.516	56.715	45.067	1 00	29.08
	ATOM	1893	CB	ALA A 2		36.112	57.464	47.121		27.40
	ATOM	1894	N	VAL A 2	2	33.502	58.608	46.197	1.00	26.51
	ATOM	1895	CA	VAL A 2		32.677	59.306	45.242		26.35
20										
20	ATOM	1896	С	VAL A 2	2	33.470	59.507	43.928	1.00	27.11
	ATOM	1897	0	VAL A 2	2	34.591	60.033	43.969	1.00	27.25
	ATOM	1898	СВ	VAL A 2	2	32.216	60.670	45.871	1.00	
	MOTA	1899	CG1	VAL A 2	2	31.510	61.532	44.897		27.60
	ATOM	1900	CG2	VAL A 2	2	31.290	60.445	47.100	1.00	25.69
25	ATOM	1901	N	ASN A 2		32.911	59.063	42.783	1.00	
23										
	ATOM	1902	CA	ASN A 2		33.526	59.241	41.456	1.00	26.59
	ATOM	1903	С	ASN A 20	3	33.094	60.531	40.841	1.00	26.64
	ATOM	1904	Ō	ASN A 2		32.046	61.067	41.206		28.69
	ATOM	1905	CB	ASN A 26	3	33.039	58.177	40.466	1.00	26.67
30	ATOM	1906	CG	ASN A 26	3	33.876	56.899	40.462	1.00	25.47
	ATOM	1907	OD1	ASN A 26		33.447	55.858	39.889		22.78
	ATOM	1908	ND2	ASN A 26	3	35.032	56.935	41.104	1.00	21.04
	ATOM	1909	N	PRO A 26	4	33.823	61.022	39.855	1.00	25.42
	ATOM	1910	CA	PRO A 26		33.356	62.186	39.104		25.26
25										
35	ATOM	1911	С	PRO A 26		32.113	61.791	38.283	1.00	25.24
	ATOM	1912	0	PRO A 26	4	31.951	60.626	37.989	1.00	24.64
	ATOM	1913	СB	PRO A 26		34.509	62.446			25.04
	ATOM	1914	CG	PRO A 26	4	35.114	61.031	37.971	1.00	25.43
	ATOM	1915	CD	PRO A 26	4	35.089	60.500	39.329	1.00	25.69
40	ATOM	1916	N	THR A 26		31.265	62.742	37.936	1.00	25.73
10										
	MOTA	1917	CA	THR A 26	5	30.099	62.489	37.086	1.00	25.58
	ATOM	1918	C	THR A 26	5	30.461	63.060	35.758	1.00	25.42
	ATOM	1919	0	THR A 26	5	31.350	63.881	35.666	1.00	24.24
			-							
	MOTA	1920	CB	THR A 26		28.841	63.211	37.588		25.82
45	ATOM	1921	OG1	THR A 26	5	29.161	64.580	37.928	1.00	26.18
	ATOM	1922	CG2	THR A 26	5	28.327	62.577	38.903	1.00	27.07
	ATOM	1923		VAL A 26		29.688	62.689	34.747		
			N						1.00	
	ATOM	1924	CA	VAL A 26	6	30.023	63.031	33.391	1.00	25.11
	ATOM	1925	С	VAL A 26	6	28.770	63.344	32.634	1.00	25.81
50	ATOM	1926		VAL A 26		27.747	62.675			25.44
50			0_					32.823		
	ATOM	1927	CB	VAL A 26	6	30.757	61.814	32.707	1.00	24.14
	ATOM	1928	CG1	VAL A 26	6	29.846	60.614	32.638	1.00	24.68
	ATOM	1929		VAL A 26		31.317		31.352		22.65
							62.168			
	ATOM	1930	N	LYS A 26	7	28.877	64.351	31.776	1.00	26.44
55	ATOM	1931	CA	LYS A 26	7	27.818	64.704	30.845	1.00	28.81
	ATOM	1932	C	LYS A 26		28.438	64.693	29.463		29.40
	ATOM	1933	0	LYS A 26	7	29.647	64.853	29.339	1.00	29.11
	ATOM	1934	CB	LYS A 26		27.266	66.090	31.154		28.26
						26.294				
	ATOM	1935	CG	LYS A 26			66.103	32.339		31.32
60	ATOM	1936	CD	LYS A 26	7	25.870	67.514	32.685	1.00	32.66
	ATOM	1937	CE	LYS A 26	7	25.259	67.592	34.075		35.71
	MOTA	1938	NZ	LYS A 26		24.396	68.825	34.141		36.32
	ATOM	1939	N	PHE A 26	8	27.598	64.533	28.440	1.00	30.61
	ATOM	1940	CA	PHE A 26		28.025	64.571	27.034		31.41
65										
65	MOTA	1941	Ç	PHE A 26		27.235	65.605	26.204		32.03
	ATOM	1942	0	PHE A 26	8	26.005	65.608	26.229	1.00	32.82
	ATOM	1943	CB	PHE A 26	8	27.838	63.204	26.411		31.30
	MOTA	1944	CG	PHE A 26		28.520	63.067	25.095		31.64
	MOTA	1945	CD1	PHE A 26	8	29.880	62.827	25.035	1.00	33.36
70	ATOM	1946	CD2	PHE A 26	8	27.819	63.247	23.923	1.00	31.47
-							 -			

5	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1947 1948 1949 1950 1951 1952	CEZ N	PHE PHE PHE PHE PHE	A 268 A 268 A 268 A 269 A 269 A 269 A 269		30.533 28.446 29.816 27.934 27.291 27.756	63.163 62.893 66.454 67.521 67.551	22.710 22.644 25.450 24.674 23.205	1.00 32.55 1.00 32.53 1.00 32.86 1.00 32.97 1.00 32.67
10	ATOM ATOM ATOM ATOM ATOM	1954 1955 1956 1957 1958	CB CG CD1 CD2 CE1	PHE PHE PHE PHE	A 269 A 269 A 269 A 269 A 269		28.879 27.638 27.269 28.134 26.047 27.801	68.890 69.041 68.658 69.584	25.279 26.719 27.703 27.087	1.00 33.14 1.00 34.68 1.00 33.64 1.00 35.51
15	ATOM ATOM ATOM ATOM ATOM ATOM	1959 1960 1961 1962 1963 1964	CE2 CZ N CA C	PHE VAL VAL VAL	A 269 A 269 A 270 A 270 A 270 A 270		25.708 26.588 26.915 27.332 27.011 25.890	69.304 68.049 68.262 69.672	28.399 29.372 22.294 20.903 20.420	1.00 35.64 1.00 33.01 1.00 32.38 1.00 32.01 1.00 32.54
20	ATOM ATOM ATOM ATOM ATOM	1965 1966 1967 1968	CG2 N	VAL VAL VAL	A 270 A 270 A 270 A 271	•	26.626 27.157 26.808 27.970	67.299 67.496 65.873 70.343	19.943 18.537 20.387 19.822	1.00 32.41 1.00 30.35 1.00 31.14 1.00 33.76
25	ATOM ATOM ATOM ATOM	1969 1970 1971 1972 1973	CA C O CB CG1	VAL VAL VAL	A 271 A 271 A 271 A 271 A 271		27.705 27.898 28.907 28.687 28.226	71.808 71.374 72.657	19.309 17.809 17.296 19.884 19.605	1.00 34.90 1.00 35.24 1.00 34.81 1.00 35.36 1.00 37.44
30	ATOM ATOM ATOM ATOM ATOM	1974 1975 1976 1977 1978	CG2 N CA C	ASN ASN ASN	A 271 A 272 A 272 A 272 A 272		28.838 26.941 27.113 27.992 27.597	72.412 72.413 72.739 73.955 75.049	21.348 17.116 15.706 15.588 15.878	1.00 36.04 1.00 36.45 1.00 37.59 1.00 38.09 1.00 37.84
35	ATOM ATOM ATOM ATOM ATOM	1979 1980 1981 1982 1983	CB CG OD1 ND2 N	ASN ASN ASN	A 272 A 272 A 272 A 272 A 273		25.803 25.973 27.064 24.920 29.189	73.040 73.130 73.491 72.752 73.691	15.001 13.501 12.980 12.785	1.00 37.83 1.00 39.15 1.00 39.51 1.00 37.38
40	ATOM ATOM ATOM ATOM ATOM	1984 1985 1986 1987 1988	CA C O CB OG1	THR THR THR THR	A 273 A 273 A 273 A 273 A 273 A 273		30.254 30.121 30.963 31.493	74.616 75.388 76.213 73.705	15.127 14.914 13.592 13.256 14.887	1.00 39.64 1.00 41.12 1.00 42.88 1.00 42.65 1.00 41.68
45	ATOM ATOM ATOM ATOM ATOM	1989 1990 1991 1992 1993	CG2 N CA C	THR ASP ASP ASP	A 273 A 274 A 274 A 274 A 274 A 274		32.322 32.345 29.089 28.940 27.976	73.920 73.930 75.113 75.871 77.009	16.053 13.693 12.804 11.565 11.802	1.00 42.46 1.00 40.87 1.00 44.51 1.00 46.51 1.00 47.68
50	ATOM ATOM ATOM ATOM ATOM	1994 1995 1996 1997 1998	CB CG OD1	ASP ASP ASP ASP	A 274 A 274 A 274 A 274 A 274 A 275		27.891 28.509 29.688 30.821 29.581	77.940 74.985 74.200 74.727 73.035	11.012 10.376 9.760 9.679 9.327	1.00 47.48 1.00 46.35 1.00 46.95 1.00 47.04 1.00 50.56
55	ATOM ATOM ATOM ATOM ATOM	1999 2000 2001 2002 2003	CA C O CB	SER A	A 275 A 275 A 275 A 275 A 275 A 275		27.314 26.278 26.606 25.736 24.982 25.106	76.966 77.928 78.783 79.040 77.173 76.433	12.947 13.251 14.462 15.279 13.516 14.709	1.00 49.96 1.00 51.76 1.00 52.74 1.00 52.56 1.00 52.07
60	ATOM ATOM ATOM ATOM ATOM	2004 2005 2006 2007 2008	N CA C O	LEU A LEU A LEU A	A 276 A 276 A 276 A 276 A 276		27.856 28.275 28.193 28.238	79.224 80.037 81.494 81.830	14.573 15.706 15.334 14.163	1.00 52.67 1.00 54.10 1.00 54.88 1.00 55.90 1.00 55.21
65	ATOM ATOM ATOM ATOM	2009 2010 2011 2012	CG CD1 CD2 N	LEU A LEU A LEU A SER A	A 276 A 276 A 276 A 277		29.721 30.014 31.507 29.372 28.107	79.723 78.312 78.087 78.054 82.344	16.110 16.617 16.693 17.954 16.351	1.00 54.72 1.00 53.97 1.00 53.31 1.00 52.74 1.00 57.26
70	ATOM ATOM ATOM ATOM	2013 2014 2015 2016	C O	SER A	A 277 A 277 A 277 A 277		28.045 28.727 28.709 26.592	83.792 84.521 84.065 84.249	16.172 17.328 18.476 16.080	1.00 58.43 1.00 59.40 1.00 59.33 1.00 58.74

	ATOM	2017	OG	SER A	277	26.380	85.378	16.898	1.00	58.81
	ATOM	2018	N	SER A	278	29.343	85.653	17.025	1.00	60.26
	ATOM	2019	CA	SER A		29.997	86.429	18.064	1.00	
	ATOM	2020	С	SER A		28.981	87.052	19.033		61.57
5	ATOM	2021	0	SER A		29.282	87.286	20.200		62.17
	ATOM	2022	СВ	SER A		30.885	87.508	17.436		61.67
	ATOM	2023	OG	SER A		30.476	87.802	16.107		61.47
	ATOM	2024	N	VAL A		27.766	87.286	18.567		61.85
10	ATOM	2025	CA	VAL A		26.763	87.921	19.412		62.09
10	ATOM	2026	C	VAL A		26.070	86.953	20.337		61.70
	ATOM	2027	O	VAL A		25.911 25.701	87.210	21.532		61.70 62.23
	ATOM ATOM	2028 2029	CB CC1	VAL A		24.411	88.615 88.787	18.563 19.336	1.00	
	ATOM	2029	CG2			26.241	89.966	18.079	1.00	
15	ATOM	2030	N N	THR A		25.635	85.845	19.770	1.00	
13	ATOM	2032	CA	THR A		24.894	84.869	20.531		60.92
	ATOM	2032	C	THR A		25.878	83.851	21.090		60.23
	ATOM	2034	ŏ	THR A		26.992	83.731	20.585	1.00	
	ATOM	2035	ČВ	THR A		23.799	84.253	19.625		61.10
20	ATOM	2036		THR A		22.619	85.069	19.702	1.00	
	ATOM	2037	CG2			23.326	82.886	20.109	1.00	61.31
	ATOM	2038	N	ASN A	281	25.480	83.163	22.160	1.00	59.15
	ATOM	2039	CA	ASN A	281	26.326	82.144	22.774	1.00	58.27
	ATOM	2040	С	ASN A	281	26.082	80.806	22.138	1.00	56.62
25	ATOM	2041	0	ASN A		24.981	80.520	21.646	1.00	
	ATOM	2042	СВ	ASN A		26.087	82.026	24.287	-	58.50
	MOTA	2043	CG	ASN A		26.765	83.121	25.071		60.33
	ATOM	2044		ASN A		27.927	83.443	24.832		62.44
20	ATOM	2045		ASN A		26.030	83.724	26.000		64.59
30	ATOM	2046 2047	N	ALA A		27.119	79.978	22.183	1.00	54.75
	ATOM	2047	CA	ALA A		27.089 26.007	78.657 77.776	21.591 22.194	1.00	53.17 51.89
	ATOM ATOM	2048	C O	ALA A		25.768	77.757	23.392	1.00	51.73
	ATOM	2050	СВ	ALA A		28.453	77.999	21.738		53.37
35	ATOM	2051	N	THR A		25.374	77.026	21.321		50.24
30	ATOM	2052	CA	THR A		24.312	76.134	21.668		49.16
	ATOM	2053	C	THR A		24.783	74.706	21.807		47.71
	ATOM	2054	Ō	THR A		24.977	74.024	20.801		48.48
	ATOM	2055	CB	THR A	283	23.342	76.147	20.524	1.00	49.07
40	ATOM	2056	OG1	THR A	283	22.738	77.439	20.434	1.00	49.95
	ATOM	2057	CG2	THR A	283	22.202	75.190	20.790	1.00	50.39
	ATOM	2058	N	SER A		24.914	74.212	23.026	1.00	
	MOTA	2059	CA	SER A		25.353	72.849	23.189		43.52
4.5	ATOM	2060	C	SER A		24.132	71.988	23.452		42.27
45	ATOM	2061	0	SER A		23.340	72.288	24.361		41.90
	ATOM	2062	CB	SER A		26.397	72.742	24.328		44.03
	ATOM	2063 2064	OG N	SER A		27.603 23.957	73.432 70.951	23.980 22.632		40.06
	ATOM ATOM	2065	N CA	ILE A		22.898	69.982	22.833		39.55
50	ATOM	2066	C	ILE A		23.412	68.790	23.658		39.06
50	ATOM	2067	ŏ	ILE A		24.395	68.138	23.293		38.89
	ATOM	2068	ČВ	ILE A		22.396	69.485	21.491		39.93
	ATOM	2069	CG1			21.833	70.649	20.671		42.07
	ATOM	2070	CG2	ILE A		21.369	68.375	21.690		39.67
55	ATOM	2071		ILE A		20.587	71.287	21.301		43.81
	ATOM	2072	N	GLN A	286	22.731	68.487	24.759	1.00	38.49
	ATOM	2073	CA	GLN A	286	23.139	67.398	25.621	1.00	37.01
	ATOM	2074	С	GLN A		22.619	66.074	25.122		36.29
	ATOM	2075	0	GLN A		21.493	65.957	24.700		35.16
60	ATOM	2076	CB	GLN A		22.630	67.616	27.055		37.50
	ATOM	2077	CG	GLN A		23.093	66.532	28.066		35.97
	ATOM	2078	CD	GLN A		22.924	66.959	29.564		38.40
	ATOM	2079	OE1			22.437	68.045	29.855		37.12
6 =	MOTA	2080	NE2	GLN A		23.323	66.089	30.482		31.63
65	ATOM	2081	N	ILE A		23.458 22.945	65.054	25.163		36.20
	ATOM ATOM	2082 2083	CA C	ILE A		22.945	63.720 63.082	24.944 26.304		35.42 35.21
	ATOM	2083	0	ILE A		24.099	62.964	26.304		35.21
	ATOM	2085	CB	ILE A		23.797	62.918	23.961		35.12
70	ATOM	2086	CG1	ILE A		23.841	63.595	22.593		35.77

ATOM 2095 CGZ THR A 288	00 35.11 00 34.90 00 34.92 00 35.17 00 35.09 00 33.84
ATOM 2100 CB ALA A 289 24 016 58:200 30.189 1.00 3 ATOM 2101 N PRO A 290 21.862 56.485 28.687 1.00 3 ATOM 2102 CA PRO A 290 20.718 55.579 28.748 1.00 3 ATOM 2103 C PRO A 290 20.152 55.447 30.159 1.00 3 ATOM 2104 O PRO A 290 20.152 55.447 30.159 1.00 3 ATOM 2105 CB PRO A 290 20.919 55.514 31.149 1.00 3 ATOM 2106 CG PRO A 290 21.320 54.224 28.386 1.00 3 ATOM 2107 CD PRO A 290 22.594 54.489 27.757 1.00 3 ATOM 2108 N ALA A 291 18.844 55.003 30.229 1.00 3 ATOM 2109 CA ALA A 291 18.144 55.033 31.497 1.00 3 ATOM 2110 C ALA A 291 18.765 53.931 32.357 1.00 3 ATOM 2111 O ALA A 291 18.765 53.931 32.357 1.00 3 ATOM 2112 CB ALA A 291 18.765 53.931 32.357 1.00 3 ATOM 2113 N SER A 292 19.261 52.896 31.704 1.00 3 ATOM 2114 CA SER A 292 19.833 51.789 32.426 1.00 3 ATOM 2115 C SER A 292 19.833 51.789 32.426 1.00 3 ATOM 2116 O SER A 292 21.222 52.115 33.015 1.00 3 ATOM 2117 CB SER A 292 19.833 51.789 32.426 1.00 3 ATOM 2117 CB SER A 292 19.803 51.709 32.426 1.00 3 ATOM 2117 CB SER A 292 19.803 51.709 32.426 1.00 3 ATOM 2118 OG SER A 292 21.748 51.355 33.823 1.00 3 ATOM 2117 CB SER A 292 21.748 51.355 33.823 1.00 3 ATOM 2112 C MET A 293 23.026 53.714 33.210 1.00 3 ATOM 2120 CA MET A 293 23.026 53.714 33.210 1.00 3 ATOM 2121 C MET A 293 23.026 53.714 33.210 1.00 3 ATOM 2120 C MET A 293 23.026 53.714 33.210 1.00 3 ATOM 2121 C MET A 293 23.026 53.714 33.210 1.00 3 ATOM 2122 C MET A 293 23.026 53.714 33.210 1.00 3 ATOM 2123 CB MET A 293 23.026 54.865 35.298 1.00 3 ATOM 2121 C MET A 293 23.026 54.865 35.298 1.00 3 ATOM 2122 C MET A 293 23.026 54.865 35.298 1.00 3 ATOM 2123 CB MET A 293 23.026 53.714 33.210 1.00 3 ATOM 2123 CB MET A 293 23.026 54.869 37.147 1.00 34 ATOM 2123 CB MET A 293 23.026 53.714 33.210 1.00 34 ATOM 2123 CB MET A 293 23.026 53.714 33.210 1.00 34 ATOM 2123 CB MET A 293 23.026 53.714 33.210 1.00 34 ATOM 2123 CB MET A 293 23.026 54.869 37.147 1.00 34 ATOM 2123 CB MET A 293 23.026 53.714 33.210 1.00 34 ATOM 2123 CB MET A 293 23.026 53.714 33.210 1.00 34 ATOM 2138 CB LEU A 294 20.688 56.878 37.093 1.00 34 ATOM 2138 CB L	00 35.05 00 36.03 00 36.30 00 35.95 00 36.76 00 37.41
ATOM 2105 CB PRO A 290 21.320 54.224 28.386 1.00 3 ATOM 2106 CG PRO A 290 22.594 54.489 27.757 1.00 3 ATOM 2108 N ALA A 291 18.844 55.200 30.229 1.00 3 ATOM 2109 CA ALA A 291 18.144 55.033 31.497 1.00 3 ATOM 2110 C ALA A 291 18.765 53.3931 32.357 1.00 3 ATOM 2111 O ALA A 291 18.765 53.931 32.357 1.00 3 ATOM 2112 CB ALA A 291 18.768 54.002 33.587 1.00 3 ATOM 2113 N SER A 292 19.261 52.896 31.704 1.00 3 ATOM 2114 CA SER A 292 19.833 51.789 32.426 1.00 3 ATOM 2115 C SER A 292 19.833 51.789 32.426 1.00 3 ATOM 2116 O SER A 292 21.748 51.355 33.823 1.00 3 ATOM 2117 CB SER A 292 21.748 51.355 33.823 1.00 3 ATOM 2118 OG SER A 292 21.748 51.355 33.823 1.00 3 ATOM 2119 N MET A 293 21.783 53.250 32.630 1.00 3 ATOM 2120 CA MET A 293 22.661 54.752 34.236 1.00 3 ATOM 2120 CA MET A 293 22.661 54.752 34.236 1.00 3 ATOM 2120 CA MET A 293 22.661 54.752 34.236 1.00 3 ATOM 2122 CG MET A 293 22.661 54.752 34.236 1.00 3 ATOM 2122 CG MET A 293 23.936 54.325 32.142 1.00 3 ATOM 2124 CG MET A 293 23.936 54.325 32.142 1.00 3 ATOM 2125 SD MET A 293 23.936 54.325 32.142 1.00 3 ATOM 2126 CE MET A 293 25.771 52.417 31.979 1.00 34 ATOM 2127 N LEU A 294 21.591 55.469 33.937 1.00 34 ATOM 2128 CA LEU A 294 21.137 56.545 34.797 1.00 34 ATOM 2130 O LEU A 294 20.009 57.315 34.105 1.00 34 ATOM 2131 CB LEU A 294 20.009 57.315 34.105 1.00 34 ATOM 2133 CD LEU A 294 20.009 57.315 34.105 1.00 34 ATOM 2133 CD LEU A 294 20.009 57.315 36.105 1.00 35 ATOM 2133 CD LEU A 294 20.009 57.315 36.105 1.00 35 ATOM 2133 CD LEU A 294 20.009 57.315 36.105 1.00 35 ATOM 2133 CD LEU A 294 20.009 57.315 36.105 1.00 35 ATOM 2133 CD LEU A 294 20.009 57.315 36.105 1.00 36 ATOM 2133 CD LEU A 294 20.009 57.315 36.105 1.00 36 ATOM 2133 CD LEU A 294 20.009 57.315 36.105 1.00 36 ATOM 2134 CD2 LEU A 294 20.009 57.315 36.105 1.00 36 ATOM 2135 N ILE A 295 20.032 54.214 37.615 1.00 36 ATOM 2136 CA ILE A 295 20.032 54.214 37.615 1.00 36 ATOM 2137 C ILE A 295 20.032 54.214 37.615 1.00 36 ATOM 2138 C ILEU A 294 20.688 56.808 37.472 1.00 39 ATOM 2134 CD2 LEU A 294 20.688 56.808 37.472 1.0	38.32 36.36 37.99 38.30 38.42
ATOM 2110 CA ALAA 291 18.144 55.033 31.497 1.00 3 ATOM 2111 O ALAA 291 18.765 53.931 32.357 1.00 3 ATOM 2111 CB ALAA 291 18.765 53.931 32.357 1.00 3 ATOM 2112 CB ALAA 291 16.661 54.713 31.231 1.00 3 ATOM 2113 N SER A 292 19.261 52.896 31.704 1.00 3 ATOM 2114 CA SER A 292 19.833 51.789 32.426 1.00 3 ATOM 2115 C SER A 292 19.833 51.789 32.426 1.00 3 ATOM 2116 O SER A 292 21.222 52.115 33.015 1.00 3 ATOM 2117 CB SER A 292 21.222 52.115 33.015 1.00 3 ATOM 2118 OG SER A 292 21.748 51.355 33.823 1.00 3 ATOM 2118 N MET A 293 21.788 53.250 32.630 1.00 3 ATOM 2119 N MET A 293 21.788 53.250 32.6630 1.00 3 ATOM 2120 CA MET A 293 23.026 53.714 33.210 1.00 3 ATOM 2121 C MET A 293 23.026 53.714 33.210 1.00 3 ATOM 2122 CMET A 293 23.026 53.714 33.210 1.00 3 ATOM 2123 CB MET A 293 23.026 53.714 33.210 1.00 3 ATOM 2124 CG MET A 293 23.026 53.714 33.210 1.00 3 ATOM 2125 SD MET A 293 23.026 53.714 33.210 1.00 3 ATOM 2124 CG MET A 293 23.026 53.714 33.210 1.00 3 ATOM 2125 CB MET A 293 23.026 53.714 33.210 1.00 3 ATOM 2124 CG MET A 293 23.026 53.714 33.210 1.00 3 ATOM 2125 CB MET A 293 23.026 53.714 33.210 1.00 3 ATOM 2124 CG MET A 293 23.026 53.714 33.210 1.00 3 ATOM 2124 CG MET A 293 23.026 53.714 33.210 1.00 3 ATOM 2124 CG MET A 293 23.026 53.714 33.210 1.00 3 ATOM 2124 CG MET A 293 23.026 53.714 33.210 1.00 3 ATOM 2124 CG MET A 293 23.026 53.714 33.210 1.00 3 ATOM 2125 CD MET A 293 23.026 54.865 35.298 1.00 3 ATOM 2125 CD MET A 293 23.026 54.865 35.298 1.00 3 ATOM 2125 CD MET A 293 23.026 54.865 35.298 1.00 3 ATOM 2127 N LEU A 294 21.591 55.469 33.937 1.00 36 ATOM 2128 CA LEU A 294 21.591 55.469 33.937 1.00 36 ATOM 2130 O LEU A 294 21.790 58.848 33.338 1.00 44 ATOM 2133 CB LEU A 294 20.014 54.795 36.322 1.00 38 ATOM 2133 CB LEU A 294 20.014 54.795 36.322 1.00 38 ATOM 2134 CD2 LEU A 294 21.790 58.848 33.338 1.00 33 ATOM 2133 CB LEU A 295 20.441 54.795 36.322 1.00 38 ATOM 2134 CD2 LEU A 294 20.705 54.505 39.912 1.00 37 ATOM 2136 CA LEU A 295 20.003 54.214 37.615 1.00 36 ATOM 2137 C ILE A 295 20.032 54.214 37.615 1.00 36 ATOM 2141	0 37.42 0 38.47 0 38.29 0 38.09 0 37.43
ATOM 2114 CA SER A 292 19.833 51.789 32.426 1.00 3 ATOM 2115 C SER A 292 21.222 52.115 33.015 1.00 3 ATOM 2116 O SER A 292 21.748 51.355 33.823 1.00 3 ATOM 2117 CB SER A 292 19.905 50.573 31.554 1.00 3 ATOM 2118 OG SER A 292 20.880 50.771 30.553 1.00 3 ATOM 2119 N MET A 293 21.783 53.250 32.630 1.00 3 ATOM 2120 CA MET A 293 23.026 53.714 33.210 1.00 3 ATOM 2121 C MET A 293 23.026 53.714 33.210 1.00 3 ATOM 2122 O MET A 293 23.026 53.714 33.210 1.00 3 ATOM 2122 O MET A 293 23.026 54.752 34.236 1.00 3 ATOM 2122 O MET A 293 23.936 54.865 35.298 1.00 3 ATOM 2122 O MET A 293 23.936 54.325 32.142 1.00 3 ATOM 2124 CG MET A 293 23.936 54.325 32.142 1.00 3 ATOM 2125 SD MET A 293 25.771 52.417 31.979 1.00 3 ATOM 2126 CE MET A 293 25.772 50.765 31.245 1.00 3 ATOM 2127 N LEU A 294 21.591 55.469 33.937 1.00 38 ATOM 2128 CA LEU A 294 21.591 55.469 33.937 1.00 38 ATOM 2129 C LEU A 294 21.591 55.469 33.937 1.00 38 ATOM 2130 O LEU A 294 20.688 56.878 37.093 1.00 33 ATOM 2131 CB LEU A 294 20.688 56.878 37.093 1.00 33 ATOM 2133 CD1 LEU A 294 20.688 56.878 37.093 1.00 33 ATOM 2133 CD1 LEU A 294 20.330 58.728 33.640 1.00 40 ATOM 2133 CD1 LEU A 294 20.330 58.728 33.640 1.00 40 ATOM 2133 CD2 LEU A 294 20.330 58.728 33.640 1.00 40 ATOM 2133 CD1 LEU A 294 20.330 58.728 33.640 1.00 40 ATOM 2133 CD1 LEU A 294 20.330 58.728 33.640 1.00 40 ATOM 2133 CD1 LEU A 294 20.330 58.728 33.640 1.00 40 ATOM 2134 CD2 LEU A 294 20.330 58.728 33.640 1.00 40 ATOM 2135 N ILE A 295 20.032 54.214 37.615 1.00 38 ATOM 2137 C ILE A 295 20.032 54.214 37.615 1.00 37 ATOM 2138 O ILE A 295 20.032 54.214 37.615 1.00 37 ATOM 2137 C ILE A 295 20.032 54.214 37.615 1.00 37 ATOM 2139 CB ILE A 295 19.642 52.060 38.802 1.00 42 ATOM 2134 CD2 LEU A 294 19.494 59.123 32.449 1.00 47 ATOM 2134 CD2 LEU A 295 19.642 52.060 38.802 1.00 42 ATOM 2134 CD2 ILE A 295 19.642 52.060 38.802 1.00 42 ATOM 2141 CG2 ILE A 295 19.642 52.060 38.802 1.00 42 ATOM 2143 N GLY A 296 22.345 54.408 38.386 1.00 36	0 37.84 0 37.19 0 36.25 0 37.87
ATOM 2119 N MET A 293 21.783 53.250 32.630 1.00 3 ATOM 2120 CA MET A 293 23.026 53.714 33.210 1.00 3 ATOM 2121 C MET A 293 22.661 54.752 34.236 1.00 3 ATOM 2122 O MET A 293 23.286 54.865 35.298 1.00 3 ATOM 2123 CB MET A 293 23.936 54.325 32.142 1.00 3 ATOM 2124 CG MET A 293 24.469 53.296 31.175 1.00 34 ATOM 2125 SD MET A 293 25.771 52.417 31.979 1.00 34 ATOM 2126 CE MET A 293 25.771 52.417 31.979 1.00 34 ATOM 2127 N LEU A 294 21.591 55.469 33.937 1.00 36 ATOM 2128 CA LEU A 294 21.591 55.469 33.937 1.00 36 ATOM 2129 C LEU A 294 20.714 56.084 36.173 1.00 36 ATOM 2130 O LEU A 294 20.688 56.878 37.093 1.00 37 ATOM 2131 CB LEU A 294 20.688 56.878 37.093 1.00 37 ATOM 2132 CG LEU A 294 20.330 58.728 33.640 1.00 40 ATOM 2133 CD1 LEU A 294 21.790 58.848 33.338 1.00 40 ATOM 2134 CD2 LEU A 294 19.494 59.123 32.449 1.00 41 ATOM 2135 N ILE A 295 20.441 54.795 36.322 1.00 38 ATOM 2136 CA ILE A 295 20.441 54.795 36.322 1.00 38 ATOM 2137 C ILE A 295 20.441 54.795 36.322 1.00 38 ATOM 2138 O ILE A 295 20.032 54.214 37.615 1.00 37 ATOM 2138 O ILE A 295 20.032 54.214 37.615 1.00 37 ATOM 2138 CB ILE A 295 20.032 54.214 37.615 1.00 37 ATOM 2138 O ILE A 295 20.032 54.214 37.615 1.00 37 ATOM 2138 O ILE A 295 20.032 54.214 37.615 1.00 37 ATOM 2138 O ILE A 295 20.032 54.214 37.615 1.00 37 ATOM 2138 O ILE A 295 20.032 54.214 37.615 1.00 37 ATOM 2138 O ILE A 295 20.032 54.214 37.615 1.00 37 ATOM 2138 O ILE A 295 20.705 54.505 39.912 1.00 37 ATOM 2139 CB ILE A 295 19.834 52.680 37.472 1.00 39 ATOM 2140 CG1 ILE A 295 19.834 52.680 37.472 1.00 39 ATOM 2141 CG2 ILE A 295 19.844 52.060 38.802 1.00 43 ATOM 2143 N GLY A 296 22.345 54.408 38.386 1.00 47	0 37.70 0 37.65 0 38.56 0 37.31
ATOM 2124 CG MET A 293 24.469 53.296 31.175 1.00 34 ATOM 2125 SD MET A 293 25.771 52.417 31.979 1.00 34 ATOM 2126 CE MET A 293 25.702 50.765 31.245 1.00 36 ATOM 2127 N LEU A 294 21.591 55.469 33.937 1.00 38 ATOM 2128 CA LEU A 294 21.137 56.545 34.797 1.00 38 ATOM 2129 C LEU A 294 20.714 56.084 36.173 1.00 38 ATOM 2130 O LEU A 294 20.688 56.878 37.093 1.00 37 ATOM 2131 CB LEU A 294 20.009 57.315 34.105 1.00 37 ATOM 2132 CG LEU A 294 20.330 58.728 33.640 1.00 40 ATOM 2133 CD1 LEU A 294 20.330 58.728 33.640 1.00 40 ATOM 2134 CD2 LEU A 294 21.790 58.848 33.338 1.00 40 ATOM 2135 N ILE A 295 20.441 54.795 36.322 1.00 38 ATOM 2136 CA ILE A 295 20.441 54.795 36.322 1.00 38 ATOM 2137 C ILE A 295 20.032 54.214 37.615 1.00 37 ATOM 2138 O ILE A 295 20.032 54.214 37.615 1.00 37 ATOM 2138 O ILE A 295 20.705 54.505 39.912 1.00 37 ATOM 2139 CB ILE A 295 19.834 52.680 37.472 1.00 37 ATOM 2139 CB ILE A 295 19.834 52.680 37.472 1.00 37 ATOM 2139 CB ILE A 295 19.834 52.680 37.472 1.00 37 ATOM 2139 CB ILE A 295 19.834 52.680 37.472 1.00 37 ATOM 2140 CG1 ILE A 295 19.834 52.680 37.472 1.00 37 ATOM 2140 CG1 ILE A 295 19.834 52.680 37.472 1.00 37 ATOM 2140 CG1 ILE A 295 19.834 52.680 37.472 1.00 37 ATOM 2140 CG1 ILE A 295 19.834 52.680 37.472 1.00 37 ATOM 2140 CG1 ILE A 295 19.834 52.680 37.472 1.00 37 ATOM 2140 CG1 ILE A 295 19.834 52.680 37.472 1.00 37 ATOM 2140 CG1 ILE A 295 19.834 52.680 37.472 1.00 37 ATOM 2140 CG1 ILE A 295 19.834 52.680 37.472 1.00 37 ATOM 2141 CG2 ILE A 295 19.834 52.680 37.472 1.00 37 ATOM 2141 CG2 ILE A 295 19.834 52.680 37.472 1.00 37 ATOM 2141 CG2 ILE A 295 19.834 52.680 37.472 1.00 37 ATOM 2141 CG2 ILE A 295 19.834 52.680 37.472 1.00 37 ATOM 2141 CG2 ILE A 295 19.834 52.680 37.472 1.00 37 ATOM 2143 N GLY A 296 22.345 54.408 38.386 1.00 36	0 37.04 0 37.24 0 37.75
ATOM 2128 CA LEU A 294 20.714 56.545 34.797 1.00 38 ATOM 2130 O LEU A 294 20.688 56.878 37.093 1.00 38 ATOM 2131 CB LEU A 294 20.009 57.315 34.105 1.00 38 ATOM 2132 CG LEU A 294 20.330 58.728 33.640 1.00 40 ATOM 2133 CD1 LEU A 294 21.790 58.848 33.338 1.00 40 ATOM 2134 CD2 LEU A 294 19.494 59.123 32.449 1.00 41 ATOM 2135 N ILE A 295 20.441 54.795 36.322 1.00 38 ATOM 2136 CA ILE A 295 20.032 54.214 37.615 1.00 38 ATOM 2137 C ILE A 295 20.032 54.214 37.615 1.00 38 ATOM 2138 O ILE A 295 20.032 54.214 37.615 1.00 38 ATOM 2138 O ILE A 295 20.032 54.214 37.615 1.00 38 ATOM 2138 O ILE A 295 20.032 54.214 37.615 1.00 37 ATOM 2139 CB ILE A 295 19.834 52.680 37.472 1.00 39 ATOM 2139 CB ILE A 295 19.834 52.680 37.472 1.00 39 ATOM 2140 CG1 ILE A 295 19.834 52.680 37.472 1.00 39 ATOM 2141 CG2 ILE A 295 19.642 52.060 38.802 1.00 42 ATOM 2142 CD1 ILE A 295 19.642 52.060 38.802 1.00 42 ATOM 2143 N GLY A 296 22.345 54.408 38.386 1.00 36	0 36.55 0 34.83 0 34.30 0 36.98 0 38.01
ATOM 2133 CD1 LEU A 294 21.790 58.848 33.338 1.00 40 ATOM 2134 CD2 LEU A 294 19.494 59.123 32.449 1.00 41 ATOM 2135 N ILE A 295 20.441 54.795 36.322 1.00 38 ATOM 2136 CA ILE A 295 20.032 54.214 37.615 1.00 39 ATOM 2137 C ILE A 295 21.062 54.413 38.743 1.00 37 ATOM 2138 O ILE A 295 20.705 54.505 39.912 1.00 37 ATOM 2139 CB ILE A 295 19.834 52.680 37.472 1.00 39 ATOM 2140 CG1 ILE A 295 18.553 52.306 36.750 1.00 43 ATOM 2141 CG2 ILE A 295 19.642 52.060 38.802 1.00 42 ATOM 2142 CD1 ILE A 295 18.528 50.744 36.416 1.00 47 ATOM 2143 N GLY A 296 22.345 54.408 38.386 1.00 36	38.65 38.03 37.83 39.32
ATOM 2138 O ILE A 295 20.705 54.505 39.912 1.00 37 ATOM 2139 CB ILE A 295 19.834 52.680 37.472 1.00 39 ATOM 2140 CG1 ILE A 295 18.553 52.306 36.750 1.00 43 ATOM 2141 CG2 ILE A 295 19.642 52.060 38.802 1.00 42 ATOM 2142 CD1 ILE A 295 18.528 50.744 36.416 1.00 47 ATOM 2143 N GLY A 296 22.345 54.408 38.386 1.00 36	0 40.48 0 41.68 0 38.36 0 39.03
ATOM 2143 N GLY A 296 22.345 54.408 38.386 1.00 36	37.90 39.30 43.56 42.21
ATOM 2144 CA GLY A 296 23.434 54.437 39.362 1.00 35 ATOM 2145 C GLY A 296 24.692 55.134 38.825 1.00 33 60 ATOM 2146 O GLY A 296 24.623 55.882 37.858 1.00 33	36.37 35.27 33.95 33.25
ATOM 2147 N ASP A 297 25.820 54.936 39.498 1.00 32 ATOM 2148 CA ASP A 297 27.074 55.508 39.067 1.00 30 ATOM 2149 C ASP A 297 27.442 54.812 37.763 1.00 29 ATOM 2150 O ASP A 297 27.265 53.631 37.670 1.00 25 ATOM 2151 CB ASP A 297 28.144 55.203 40.111 1.00 31	30.86 29.01 25.96
ATOM 2152 CG ASP A 297 28.157 56.201 41.278 1.00 32 ATOM 2153 OD1 ASP A 297 27.575 57.306 41.204 1.00 37 ATOM 2154 OD2 ASP A 297 28.762 55.951 42.305 1.00 34 ATOM 2155 N HIS A 298 27.969 55.541 36.779 1.00 28 70 ATOM 2156 CA HIS A 298 28.365 54.930 35.500 1.00 28	32.76 37.01 34.16 28.26

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55.729
56.742
      ATOM
               2157
                      C
                           HIS A 298
                                             29.514
                                                                           1.00 27.63
                                                                 34.923
              2158
                           HIS A 298
     ATOM
                      0
                                             29.873
                                                                                 28.58
                                                                 35.468
                                                                           1.00
                                             27.179
     ATOM
              2159
                      CB
                           HIS A 298
                                                       54.959
                                                                 34.509
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     ATOM
              2160
                           HIS A 298
                                                       56.293
                      CG
                                             26.509
                                                                 34.465
                                                                           1.00 27.81
     ATOM
                           HIS A 298
              2161
                      ND1
                                             26.917
                                                       57.296
                                                                 33.617
                                                                           1.00 24.43
                                                                          1.00 25.10
1.00 25.84
     ATOM
              2162
                      CD2
                           HIS A 298
                                             25.492
                                                       56.805
                                                                 35.197
                                             26.214
                          HIS A 298
                                                       58.387
     MOTA
              2163
                      CE1
                                                                 33.858
     ATOM
              2164
                      NE2 HIS A 298
                                             25.318
                                                       58.108
                                                                 34.792
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                                             30.090
     ATOM
              2165
                           TYR A 299
                     N
                                                       55.266
                                                                 33.825
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     ATOM
              2166
                      CA
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                                                       55.984
                                                                 33.129
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     ATOM
              2167
                      С
                                                       56.134
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32.469
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              2168
                     0
                           TYR A 299
                                                       55.308
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                                                       55.170
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     ATOM
              2170
                     CG
                           TYR A 299
                                             32.962
                                                       54.739
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34.892
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                          TYR A 299
                                             33.572
     ATOM
              2171
                     CD1
                                                       55.650
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              2172
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CD2 LEU A 300
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TRP A 305
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	ATOM ATOM	2227 2228		ALA A 30		30.276			
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	ATOM	2230		ALA A 30		30.404			
5		2231		ALA A 30		28.815	55.731	13.085	
	ATOM	2232		THR A 30		29.059			
	MOTA ATOM	2233 2234		THR A 30		28.962			
	ATOM	2235	Ö	THR A 30		28.993 29.299		10.442 11.579	
10		2236	ČВ	THR A 30		27.666		9.381	
	ATOM	2237	OG:			26.562		10.150	
	ATOM	2238	CG			27.441		9.275	1.00 34.16
	ATOM ATOM	2239 2240	N	GLN A 30		28.675		9.456	1.00 36.94
15	ATOM	2240	CA C	GLN A 30 GLN A 30		28.595 27.472	62.746 63.119	9.610	1.00 36.92
	ATOM	2242	Ö	GLN A 30		27.420		10.560 11.084	1.00 37.03 1.00 37.35
	MOTA	2243	СВ	GLN A 30		28.337	63.443	8.245	1.00 37.33
	MOTA	2244	CG	GLN A 30		29.417	63.194	7.140	1.00 38.17
20	MOTA	2245	CD	GLN A 30		30.813	63.689	7.546	1.00 42.65
20	ATOM ATOM	2246 2247	OE1 NE2			30.954	64.550	8.441	1.00 43.08
	ATOM	2248	N	GLU A 30		31.850 26.567	63.123 62.183	6.918 10.805	1.00 40.49 1.00 36.71
	ATOM	2249	CA	GLU A 30		25.377	62.488	11.575	1.00 35.71
	ATOM	2250	С	GLU A 30	9	25.050	61.421	12.602	1.00 34.91
25	ATOM	2251	0	GLU A 30		23.963	61.416	13.167	1.00 35.07
	ATOM ATOM	2252 2253	CB	GLU A 30		24.191	62.676	10.594	1.00 36.50
	ATOM	2254	CG CD	GLU A 30:		24.558 23.413	63.640 64.366	9.472 8.766	1.00 36.43 1.00 39.46
	ATOM	. 2255	OE1			22.199	64.156	9.081	1.00 39.46 1.00 34.63
30	MOTA	2256	OE2		9	23.785	65.180	7.854	1.00 34.03
	ATOM	2257	N	ARG A 31		25.974	60.508	12.858	1.00 33.71
	ATOM ATOM	2258 2259	CA	ARG A 310		25.690	59.428	13.769	1.00 33.41
	ATOM	2259	C O	ARG A 310		26.826 27.982	59.287 59.203	14.765 14.356	1.00 33.15
35	ATOM	2261	СВ	ARG A 310		25.538	58.154	12.972	1.00 32.29 1.00 33.68
	ATOM	2262	CG	ARG A 310		25.274	56.893	13.777	1.00 36.39
	ATOM	2263	CD	ARG A 310		24.660	55.779	12.922	1.00 39.54
	ATOM ATOM	2264	NE	ARG A 310		23.250	55.583	13.231	1.00 43.09
40	ATOM	2265 2266	CZ NH1	ARG A 310		22.353 22.686	55.034	12.434	1.00 46.21
	ATOM	2267	NH2			21.089	54.636 54.925	11.224 12.845	1.00 48.82 1.00 47.65
	MOTA	2268	N	ILE A 311		26.494	59.243	16.055	1.00 47.03
	MOTA	2269	CA	ILE A 311		27.511	59.117	17.115	1.00 34.40
45	MOTA MOTA	2270 2271	C	ILE A 311		27.264	57.868	17.923	1.00 33.36
43	ATOM	2271	O CB	ILE A 311 ILE A 311		26.146 27.532	57.573	18.313	1.00 33.46
	ATOM	2273		ILE A 311		27.332	60.338 61.662	18.101 17.375	1.00 34.77 1.00 37.84
	ATOM	2274	CG2	ILE A 311		28.825	60.388		1.00 37.84
50	ATOM	2275	CD1	ILE A 311		26.952	62.833	18.302	1.00 39.22
50	ATOM ATOM	2276 2277	N	SER A 312		28.327	57.140	18.197	1.00 32.30
	ATOM	2278	CA C	SER A 312 SER A 312		28.213 28.804	55.957 56.335	19.042	1.00 32.09
	ATOM	2279	Õ	SER A 312		29.871	56.919	20.395 20.425	1.00 31.13 1.00 30.12
	ATOM	2280	CB	SER A 312		29.020	54.844	18.416	1.00 30.12
55	MOTA	2281	OG	SER A 312		28.961	53.709	19.195	1.00 32.79
	ATOM	2282	N	LEU A 313		28.095	56.053	21.485	1.00 30.37
	ATOM ATOM	2283	CA	LEU A 313		28.612	56.297	22.837	1.00 31.25
	ATOM	2284 2285	C 0	LEU A 313 LEU A 313		28.550 27.451	55.006	23.623	1.00 30.83
60	ATOM	2286	СВ	LEU A 313		27.777	54.441 57.335	23.718 23.584	1.00 31.63 1.00 30.44
	ATOM	2287	CG	LEU A 313		27.584	58.683	22.918	1.00 30.44
	MOTA	2288	CD1	LEU A 313		26.682	59.541	23.773	1.00 32.34
	ATOM	2289		LEU A 313		28.908	59.377	22.685	1.00 34.95
65	ATOM	2290	N	GLN A 314		29.686	54.520	24.148	1.00 30.07
65	ATOM ATOM	2291 2292	CA C	GLN A 314 GLN A 314		29.689	53.350	25.021	1.00 30.67
	ATOM	2293	0	GLN A 314 GLN A 314		29.751 30.629	53.818 54.604	26.476	1.00 28.79
	ATOM	2294	СВ	GLN A 314		30.871	52.388	26.841 24.791	1.00 28.37 1.00 31.25
	ATOM	2295	CG	GLN A 314		30.608	51.259	23.849	1.00 31.25
70	ATOM	2296	CD	GLN A 314		31.550	50.026	24.008	1.00 37.43

	ATOM	2297	OE1	GLN A	314	31.070	48.894	24.133	1.00 40.38
	ATOM	2298		GLN A		32.862	50.247	23.920	1.00 40.87
	ATOM	2299	N		315	28.880	53.258	27.298	1.00 28.07
	ATOM	2300	CA		315	28.799	53.572	28.714	1.00 27.91
5	ATOM	2301	С		315	28.931	52.310	29.508	1.00 27.90
	ATOM	2302	0		315	28.627	51.256	28.997	1.00 26.86
	MOTA	2303	CB	TRP A	315	27.465	54.183	29.098	1.00 27.41
	MOTA	2304	CG		315	27.037	55.330	28.340	1.00 27.24
	MOTA	2305	CD1	TRP A	315	26.389	55.330	27.128	1.00 28.62
10	ATOM	2306	CD2	TRP A	315	27.125	56.681	28.737	1.00 27.34
	MOTA	2307	NE1	TRP A	315	26.091	56.609	26.753	1.00 25.10
	MOTA	2308		TRP A		26.530	57.457	27.729	1.00 25.13
	MOTA	2309	CE3	TRP A	315	27.656	57.332	29.853	1.00 26.34
	ATOM	2310	CZ2	TRP A	315	26.487	58.815	27.790	1.00 26.49
15	MOTA	2311	CZ3	TRP A	315	27.591	58.674	29.915	1.00 24.80
	ATOM	2312	CH2	TRP A	315	27.019	59.408	28.896	1.00 26.78
	ATOM	2313	N	LEU A	316	29.341	52.436	30.786	1.00 27.28
	ATOM	2314	CA	LEU A	316	29.622	51.274	31.623	1.00 27.37
	ATOM	2315	С	LEU A		29.134	51.583	33.017	1.00 26.51
20	ATOM	2316	0	LEU A		29.402	52.667	33.511	1.00 24.17
	ATOM	2317	CB	LEU A		31.138	51.125	31.756	1.00 27.59
	ATOM	2318	CG	LEU A		31.977	49.849	31.837	1.00 29.63
	ATOM	2319		LEU A		33.388	50.130	32.427	1.00 27.30
	ATOM	2320	CD2	LEU A		31.328	48.722	32.500	1.00 30.98
25	ATOM	2321	N	ARG A		28.488	50.623	33.651	1.00 26.17
	ATOM	2322	CA	ARG A		28.050	50.814	35.007	1.00 29.17
	ATOM	2323	С	ARG A		29.274	50.717	35.931	1.00 29.53
	ATOM	2324	0	ARG A		30.220	50.025	35.624	1.00 30.93
	MOTA	2325	CB	ARG A		27.082	49.738	35.393	1.00 28.87
30	MOTA	2326	CG	ARG A		25.693	49.932	34.913	1.00 31.02
	MOTA	2327	CD	ARG A		24.699	48.952	35.588	1.00 33.50
	ATOM	2328	NE	ARG A		23.383	49.133	35.025	1.00 38.70
	ATOM	2329	CZ	ARG A		22.459	48.190	34.950	1.00 41.63
25	ATOM	2330		ARG A		22.688	46.961	35.416	1.00 40.89
35	ATOM	2331		ARG A		21.299	48.482	34.390	1.00 41.28
	ATOM	2332	N	ARG A		29.267	51.436	37.028	1.00 30.66
	ATOM	2333	CA	ARG A		30.347	51.342	38.009	1.00 31.11
	ATOM	2334	C	ARG A		30.624	49.893	38.414	1.00 31.80
40	ATOM	2335 2336	O	ARG A		31.767 30.023	49.506 52.190	38.617 39.224	1.00 31.07 1.00 31.69
40	ATOM ATOM	2337	CB CG	ARG A		31.204	52.190	40.138	1.00 31.09
	ATOM	2338	CD	ARG A		31.040	53.395	41.175	1.00 29.33
	ATOM	2339	NE	ARG A		32.171	53.368	42.092	1.00 29.21
	ATOM	2340	CZ	ARG A		32.517	54.357	42.906	1.00 30.35
45	ATOM	2341		ARG A		31.801	55.464	42.957	1.00 28.27
	ATOM	2342		ARG A		33.596	54.228	43.686	1.00 30.41
	ATOM	2343	N	ILE A		29.589	49.085	38.566	1.00 33.43
	ATOM	2344	CA	ILE A		29.831	47.650	38.626	1.00 34.95
	ATOM	2345	Ċ	ILE A		30.090	47.290	37.171	1.00 35.08
50	ATOM	2346	ŏ	ILE A		29.178	47.125	36.365	1.00 34.25
	ATOM	2347	СB	ILE A		28.662	46.854	39.188	1.00 35.85
	ATOM	2348	CG1			28.281	47.352	40.575	1.00 40.14
	ATOM	2349	CG2	ILE A	319	29.108	45.402	39.371	1.00 38.30
	ATOM	2350	CD1	ILE A		27.121	46.470	41.213	1.00 44.56
55	ATOM	2351	N	GLN A		31.357	47.171	36.829	1.00 35.11
	ATOM	2352	CA	GLN A	320	31.736	47.069	35.452	1.00 35.60
	MOTA	2353	С	GLN A	320	31.364	45.712	34.795	1.00 36.40
	ATOM	2354	0	GLN A	320	32.186	45.096	34.097	1.00 35.91
	ATOM	2355	CB	GLN A	320	33.207	47.403	35.386	1.00 35.70
60	ATOM	2356	CG	GLN A	320	33.477	48.794	35.908	1.00 34.45
	MOTA	2357	CD	GLN A		34.925	49.180	35.785	1.00 34.19
	MOTA	2358	OE1	GLN A		35.591	48.778	34.839	1.00 33.00
	MOTA	2359	NE2	GLN A		35.415	49.990	36.727	1.00 30.75
	ATOM	2360	N	ASN A		30.103	45.303	35.020	1.00 36.78
65	ATOM	2361	CA	ASN A		29.532	44.058	34.497	1.00 37.33
	MOTA	2362	C	ASN A		28.406	44.271	33.469	1.00 36.63
	MOTA	2363	0	ASN A		27.810	43.295	33.003	1.00 36.78
	ATOM	2364	СВ	ASN A		28.996	43.127	35.629	1.00 37.05
	MOTA	2365	CG	ASN A		27.778	43.677	36.385	1.00 40.00
70	MOTA	2366	ODI	ASN A	321	27.238	44.766	36.135	1.00 43.74

5	ATOM ATOM ATOM ATOM ATOM	2367 2368 2369 2370 2371	N CA C	TYR TYR	A 322 A 322 A 322	27.341 28.133 27.088 27.468	45.528 45.850 47.149	33.125 32.197 31.455	1.00 35.10 1.00 34.16 1.00 33.35
J	ATOM ATOM ATOM	2372 2373 2374	CB CG CD1	TYR TYR L TYR	A 322 A 322 A 322 A 322	27.757 25.785 24.508 24.048	45.988 46.086 47.306	33.007 32.191 31.748	1.00 33.91 1.00 35.53 1.00 34.64
10	ATOM ATOM	2375 2376 2377 2378	CEI CEI CZ	TYR TYR TYR	A 322 A 322 A 322 A 322	23.745 22.907 22.593 22.179	47.406 45.057 46.282	31.082 31.236 30.804	1.00 35.86 1.00 35.40 1.00 37.49
15	ATOM ATOM ATOM ATOM ATOM	2379 2380 2381 2382	OH N CA C	SER . SER .	A 322 A 323 A 323 A 323	21.008 27.517 27.810 26.816	47.104 48.283 48.444	30.126 29.315 28.215	1.00 32.85 1.00 32.99 1.00 32.86
20	ATOM ATOM ATOM ATOM ATOM	2383 2384 2385 2386 2387	O CB OG N	SER A SER A VAL A	A 323 A 323 A 323 A 324	26.299 29.175 29.331 26.584	48.177 46.915 49.673	28.647 28.052 27.822	1.00 32.06 1.00 33.46 1.00 35.41 1.00 33.68
25	ATOM ATOM ATOM ATOM	2388 2389 2390 2391	CA C O CB CG1	VAL A VAL A	A 324 A 324 A 324 A 324	25.597 26.176 26.716 24.380	49.916 50.801 51.870 50.610	26.828 25.759 26.050 27.434	1.00 34.23 1.00 34.59 1.00 34.10 1.00 34.28
23	ATOM ATOM ATOM ATOM	2392 2393 2394 2395	CG2 N CA C	VAL A MET A MET A	A 324 A 325 A 325	23.463 23.605 26.021 26.384	51.091 49.672 50.353 51.140	26.331 28.402 24.519 23.367	1.00 35.67 1.00 34.51 1.00 35.21 1.00 36.29
30	ATOM ATOM ATOM ATOM	2396 2397 2398 2399	O CB CG	MET A MET A MET A	325 325 325	25.102 24.146 26.995 28.170	51.785 51.079 50.268 50.923	22.865 22.504 22.262 21.505	1.00 36.58 1.00 36.39 1.00 36.35 1.00 38.37
35	ATOM ATOM ATOM ATOM	2400 2401 2402	SD CE N CA	MET A MET A ASP A ASP A	325 326 326	28.923 27.992 25.095 24.010	49.807 50.257 53.119 53.917	20.259 18.898 22.875 22.341	1.00 42.06 1.00 36.19 1.00 36.53 1.00 36.73
40	ATOM ATOM ATOM ATOM ATOM	2403 2404 2405 2406 2407 2408	C O CB CG OD1 OD2	ASP A ASP A ASP A ASP A ASP A	326 326 326 326	24.376 25.490 23.785 22.371 21.773	54.427 54.847 55.118 55.262 54.229	20.980 20.759 23.215 23.618 23.962	1.00 36.99 1.00 37.13 1.00 37.30 1.00 39.85
45	ATOM ATOM ATOM ATOM	2409 2410 2411 2412	N CA C O	ILE A ILE A ILE A	327 327 327 327	21.762 23.433 23.671 22.793 21.605	56.357 54.411 54.939 56.160 56.040	23.611 20.052 18.732 18.535 18.493	1.00 44.95 1.00 37.51 1.00 38.16 1.00 38.52 1.00 38.42
50	ATOM ATOM ATOM ATOM ATOM	2414 2415 2416 2417	CB CG1 CG2 CD1 N	ILE A ILE A ILE A CYS A	327 327 327	23.373 24.494 23.305 24.109 23.387	53.832 52.804 54.383 51.511 57.326	17.703 17.757 16.298 17.098 18.340	1.00 38.43
55	ATOM ATOM ATOM ATOM ATOM ATOM	2418 2419 2420 2421 2422 2423		CYS A CYS A CYS A CYS A CYS A ASP A	328 328 328 328 328	22.631 22.714 23.804 23.174 23.240 21.563	58.571 59.309 59.495 59.487 58.708 59.793	18.312 16.993 16.454 19.406 21.027 16.517	1.00 39.97 1.00 40.41 1.00 39.69 1.00 40.48 1.00 42.44
60	ATOM ATOM ATOM	2424 2425 2426 2427	CA C O CB	ASP A ASP A ASP A	329 329 329 329	21.473 20.974 20.119 20.520	60.435 61.877 62.198 59.611	15.213 15.270 16.058 14.334	1.00 40.89 1.00 41.39 1.00 41.92 1.00 40.55 1.00 41.65
65	ATOM ATOM ATOM ATOM ATOM ATOM	2428 2429 2430 2431 2432 2433	OD1 OD2 N CA	ASP A ASP A ASP A TYR A TYR A TYR A	329 329 330 330	21.078 22.316 20.361 21.539 21.146 19.844	58.250 58.073 57.295 62.732 64.118 64.297	13.997 13.960 13.707 14.425 14.330 13.567	1.00 42.09 1.00 42.62 1.00 45.91 1.00 43.37 1.00 45.55 1.00 47.23
70	ATOM ATOM ATOM		O CB	TYR A TYR A TYR A	330 330	19.696 22.215 21.989	63.790 64.872 66.358	12.479 13.563 13.397	1.00 46.53 1.00 45.86 1.00 46.44

	ATOM ATOM ATOM	2437 2438 2439	CD1 CD2 CE1		A	330	21.957 21.851 21.776		67.204 66.924 68.566	14.488 12.143 14.330	1.00	47.55 48.93 47.61
5	ATOM ATOM ATOM	2440 2441	CE2 CZ	TYR	Α		21.671 21.645		68.295 69.100	11.983 13.080	1.00	47.43 47.48
	ATOM ATOM	2442 2443	OH N	ASP	Α	330 331	21.491 18.906	5	70.454 65.025	12.931 14.146	1.00	49.37 50.39
10	ATOM ATOM ATOM	2444 2445 2446	CA C O	ASP ASP ASP	A		17.643 17.730 17.660)	65.331 66.709 67.719	13.482 12.850 13.541	1.00	52.45 54.21 53.88
10	ATOM ATOM	2447 2448	CB CG	ASP ASP	Α	331	16.516 15.175	;	65.328 65.672	14.492 13.863	1.00	52.85 53.55
	ATOM ATOM	2449 2450		ASP	Α	331	15.157 14.103		66.349 65.314	12.798 14.385	1.00	55.91 51.08
15	ATOM ATOM ATOM	2451 2452 2453	N CA	GLU GLU GLU	Α	332	17.851 18.076 17.075	i	66.743 67.986 69.081	11.528 10.804 11.142	1.00	56.40 58.14 58.88
	ATOM ATOM	2454 2455	C O CB	GLU GLU	Α	332	17.434 18.019	. '	70.247 67.716	11.216	1.00	59.23 58.97
20	ATOM ATOM	2456 2457	CG CD	GLU	Α	332	18.910 18.759		68.617 68.313	8.460 6.972	1.00	61.14 64.90
	ATOM ATOM	2458 2459	OE1 OE2	GLU	Α	332	18.225 19.156		67.222 69.164	6.643 6.132	1.00	66.07
25	ATOM ATOM	2460 2461	N CA	SER SER	Α	333	15.813 14.809	+	68.722 69.746	11.323 11.558	1.00	59.70 60.31
	MOTA MOTA	2462 2463	C 0	SER SER	A	333	14.873 15.106	•	70.137 71.291	13.026 13.356	1.00	60.35 60.53
20	ATOM ATOM	2464 2465	CB OG	SER SER	Α	333	13.410		69.256 68.607	11.160 12.238	1.00	60.41
30	ATOM ATOM ATOM	2466 2467 2468	N CA C	SER SER SER	A	334	14.721 14.773 16.047	(69.149 69.363 70.059	13.894 15.330 15.751	1.00	60.21 60.35 59.88
	ATOM ATOM	2469 2470	O CB	SER SER	A	334	16.044 14.699	•	70.869 68.013	16.662 16.035	1.00	60.48
35	ATOM ATOM	2471 2472	OG N	SER GLY	Α	334	14.620 17.141	(68.147 69.740	17.435 15.074	1.00	61.75 59.42
	ATOM ATOM	2473 2474	CA C	GLY GLY	Α	335	18.452 19.000		70.221 69.388	15.452 16.602	1.00	58.81 58.03
40	ATOM ATOM	2475 2476	O N	GLY ARG	Α	336	20.082	(69.665 68.349	17.119 16.991	1.00	58.62 57.08
	ATOM ATOM ATOM	2477 2478 2479	CA C O	ARG ARG ARG	Α	336	18.621 19.324 19.731	(67.551 56.225 55.982	18.169 17.858 16.721	1.00	56.39 54.43 53.58
45	ATOM ATOM	2480 2481	CB CG	ARG ARG	Α	336	17.360 16.756	(57.309 58.602	19.006 19.551	1.00	57.25 59.72
10	ATOM ATOM	2482 2483	CD NE	ARG ARG	Α	336	15.922 15.666	(58.451 59.766	20.822	1.00	63.58 66.15
	ATOM ATOM	2484 2485		ARG ARG	A A	336 336	16.409 17.474		70.339 59.728	22.375 22.900	1.00	66.97
50	ATOM ATOM	2486 2487	N	ARG TRP	Α	337	16.068 19.498	•	71.542	22.816 18.891	1.00	69.67 52.10
	ATOM ATOM	2488 2489 2490	CA C	TRP	Α	337	20.141 19.307 18.958	•	54.088 53.065 53.240	18.749 19.457 20.617	1.00	50.39 50.29 50.80
55	ATOM ATOM ATOM	2491 2492	O CB CG	TRP TRP TRP	Α	337	21.549 22.502	6	54.062 54.856	19.358 18.613	1.00	49.01 43.93
	ATOM ATOM	2493 2494		TRP	Α	337	22.748 23.372	6	66.176 54.403	18.766 17.582	1.00	41.17
60	MOTA MOTA	2495 2496	NE1 CE2	TRP TRP	A	337	23.704 24.103	6	56.586 55.510	17.874 17.135	1.00	38.20 37.28
	ATOM ATOM	2497 2498	CZ2	TRP	Α	337	23.565 25.012	6	53.182 55.429	16.945 16.112	1.00	36.08 36.93
6 5	ATOM ATOM	2499 2500	CH2	TRP	Α	337	24.475 25.192	6	53.106 54.215	15.948 15.539	1.00	35.12 35.09
65	ATOM ATOM ATOM	2501 2502 2503	N CA C	ASN ASN ASN	Α	338	19.013 18.151 18.782	6	51.974 50.966 59.601	18.777 19.360 19.364	1.00	50.08 50.17 49.12
	ATOM ATOM	2504 2505	O CB	ASN ASN	Α	338	19.398 16.798	5	59.184 50.955	18.387 18.644	1.00	49.12 49.10 50.84
70	ATOM	2506	CG	ASN			15.967		52.160	19.000		52.32

	ATOM ATOM ATOM ATOM	2507 2508 2509 2510	ND2 N	ASN CYS	A 338 A 338 A 339 A 339	15.284 16.045 18.623 19.275	63.201 58.912	18.179 20.476	1.00	56.68 53.70 48.04 48.30
5	ATOM ATOM ATOM ATOM	2511 2512 2513 2514	C O CB SG	CYS CYS CYS	A 339 A 339 A 339 A 339	18.170 17.597 20.288 21.401	56.619 56.548 57.722	20.904 21.980 21.818	1.00 1.00 1.00	48.30 49.07 48.71 47.82 45.14
10	ATOM ATOM ATOM ATOM	2515 2516 2517 2518	N CA C O	LEU LEU	A 340 A 340 A 340 A 340	17.901 16.809 17.090 17.987	55.818 54.885 53.745	19.887 19.929 20.865 20.633	1.00 1.00 1.00	49.54 50.67 50.43
15	ATOM ATOM ATOM ATOM	2519 2520 2521 2522	CG CD1 CD2	LEU LEU	A 340 A 340 A 340 A 340	16.528 15.056 14.381 14.893	54.366 54.371 55.656 54.230	18.521 18.159 18.678 16.644	1.00 1.00 1.00	50.91 52.84 53.31 52.52
20	ATOM ATOM ATOM ATOM ATOM	2523 2524 2525 2526 2527	N CA C O CB	VAL VAL VAL	A 341 A 341 A 341 A 341 A 341	16.275 16.533 16.639 17.201 15.446	52.631 51.283 50.365	21.904 22.944 22.296 22.881 24.097	1.00 1.00 1.00	51.21 51.79 52.02 51.85
25	ATOM ATOM ATOM ATOM	2528 2529 2530 2531	CG1	VAL VAL ALA	A 341 A 341 A 342 A 342	16.020 14.913 16.155 16.142	52.121 54.043 51.182 49.910	25.412 24.351 21.055 20.326	1.00 1.00 1.00	52.37 52.37 53.02 52.45 52.38
20	ATOM ATOM ATOM ATOM	2532 2533 2534 2535	C O CB N	ALA ALA ARG	A 342 A 342 A 342 A 343	17.364 17.554 14.890 18.184	49.561 48.368 49.817 50.517	19.496 19.164 19.452 19.055	1.00 1.00 1.00	52.19 53.38 53.05 50.99
30	ATOM ATOM ATOM ATOM ATOM	2536 2537 2538 2539	CA C O CB	ARG ARG ARG	A 343 A 343 A 343 A 343	19.453 20.516 21.673 19.980	50.013 49.891 49.616 50.735	18.508 19.622 19.353 17.255	1.00 1.00 1.00	49.82 47.74 47.28 49.82
35	ATOM ATOM ATOM ATOM	2540 2541 2542 2543 2544	CG CD NE CZ	ARG ARG	A 343 A 343 A 343 A 343 A 343	20.200 19.170 19.158 18.601	52.183 52.981 52.772 53.611	17.356 16.676 15.245 14.391	1.00 1.00 1.00	50.27 51.54 51.73 51.85
40	ATOM ATOM ATOM ATOM	2545 2546 2547 2548	NH2 N CA	ARG AGLN AGLN	A 343 A 344 A 344 A 344	18.023 18.637 20.114 21.075 21.723	54.705 53.363 50.055 49.932 48.582	14.840 13.086 20.875 21.967 21.927	1.00 1.00 1.00	48.59 54.27 46.47 44.89 44.26
45	ATOM ATOM ATOM ATOM	2549 2550 2551 2552	O CB CG CD	GLN A GLN A GLN A	A 344 A 344 A 344 A 344	21.055 20.408 20.271 19.672	47.590 50.082 51.483 51.530	21.800 23.318 23.815 25.190	1.00 1.00 1.00	44.26 43.75 44.84 43.22 44.80
50	ATOM ATOM ATOM ATOM ATOM	2553 2554 2555 2556 2557	NE2 N CA	GLN A HIS A HIS A	A 344 A 344 A 345 A 345 A 345	19.569 19.263 23.036 23.655 24.208	50.492 52.732 48.526 47.223 47.031	25.868 25.619 21.989 22.119 23.533	1.00 1.00 1.00	42.35 43.12 43.91 44.32
55	ATOM ATOM ATOM ATOM ATOM	2558 2559 2560 2561 2562	O CB CG ND1 I CD2 I	HIS A HIS A HIS A HIS A	A 345 A 345 A 345 A 345 A 345	24.812 24.701 24.118 23.849 23.717	47.927 47.022 46.552 47.406 45.321	24.104 21.049 19.758 18.709 19.359	1.00 1.00 1.00 1.00	43.74 43.43 44.71 46.48 50.06 47.51
60	ATOM ATOM ATOM ATOM ATOM	2563 2564 2565 2566 2567	CA :	HIS A HIS A ILE A ILE A ILE A	345 346 346	23.335 23.250 24.010 24.321 25.406	46.714 45.445 45.839 45.533 44.498	17.704 18.071 24.068 25.456 25.572	1.00 1.00 1.00 1.00	50.97 49.88 44.11 44.80 44.66
65	ATOM ATOM ATOM ATOM ATOM	2568 2569 2570 2571 2572	O : CB : CG1 :	ILE A ILE A ILE A ILE A	346 346 346 346	25.445 23.061 21.984 23.403	43.579 44.957 46.030 44.349	24.782 26.130 26.251 27.485	1.00 1.00 1.00 1.00	44.38 45.03 46.42 45.11
70	ATOM ATOM ATOM ATOM	2572 2573 2574 2575 2576	N CA C	GLU A GLU A GLU A GLU A	347 347 347	20.698 26.281 27.304 27.319 27.265	45.504 44.647 43.634 43.349 44.287	26.887 26.561 26.846 28.332 29.130	1.00 1.00 1.00 1.00	44.63 45.49 46.21

	3 moss	2577		a	247	20		44 400				
	ATOM	2577	CB	GLU A			683	44.102		431		45.45
	ATOM	2578	CG	GLU A	-		840	44.218		941	1.00	
	ATOM	2579	CD	GLU A			230	44.657	24.	535	1.00	46.13
	ATOM	2580	OE1	l GLU A	347	31.	228	44.114	25.	070	1.00	44.42
5	ATOM	2581	OE2	GLU A	347	30.	305	45.522	23.	641	1.00	48.13
	ATOM	2582	N	MET A	348	27.	383	42.064	28.	692	1.00	46.97
	ATOM	2583	CA	MET A	348		417	41.624		080		47.81
	ATOM	2584	C	MET A			436	40.512				48.11
	ATOM	2585	ŏ	MET A			596	39.690			1.00	
10	ATOM	2586	СВ	MET A		26.						
10								41.037			1.00	
	ATOM	2587	CG	MET A			850	41.803			1.00	
	ATOM	2588	SD	MET A		23.		41.001			1.00	
	ATOM	2589	CE	MET A		23.		39.227	30.	232	1.00	58.62
	MOTA	2590	N	SER A	349	29.	153	40.449	31.	319	1.00	48.36
15	ATOM	2591	CA	SER A	349	30.	059	39.325	31.	465	1.00	48.44
	ATOM	2592	С	SER A	349	29.		38.520				48.12
	ATOM	2593	ō	SER A		28.		39.068				48.86
	ATOM	2594	ČВ	SER A		31.		39.739			1.00	
	ATOM	2595	OG	SER A		32.		38.621			1.00	
20	ATOM	2596		THR A		29.						
20			N					37.214			1.00	
	ATOM	2597	CA	THR A		29.		36.342			1.00	
	ATOM	2598	C	THR A		30.		36.049				46.74
	ATOM	2599	0	THR A		30.3		36.207			1.00	
	ATOM	2600	CB	THR A	350	28.	503	35.029	32.	918	1.00	48.52
25	ATOM	2601	OG1	THR A	350	27.0	077	35.036	33.	128	1.00	48.99
	ATOM	2602	CG2	THR A	350	28.9	935	33.779	33.	680		49.06
	ATOM	2603	N	THR A		31.		35.668	33.			44.97
	ATOM	2604	CA	THR A		32.5		35.220			1.00	
	ATOM	2605	Č	THR A		33.9		36.322	35.			42.20
30	ATOM	2606	ŏ	THR A		34.3						
50								36.049			1.00	
	ATOM	2607	CB	THR A		33.3		34.161	33.			44.01
	ATOM	2608	OG1			33.7		34.647				43.68
	ATOM	2609		THR A		32.4		32.935	33.			43.10
	ATOM	2610	N	GLY A		33.2		37.575	34.	338	1.00	40.20
35	ATOM	2611	CA	GLY A	352	34.1	104	38.652	35.2	275	1.00	37.56
	ATOM	2612	С	GLY A	352	33.6	645	40.018	34.8	328	1.00	35.69
	ATOM	2613	0	GLY A	352	32.4	492	40.400	35.0		1.00	33.74
	ATOM	2614	N	TRP A		34.5		40.757	34.			32.99
	ATOM	2615	CA	TRP A		34.2		42.148	33.8			31.53
40	ATOM	2616	C	TRP A		34.1		42.268	32.3			30.70
40		2617										
	ATOM		0	TRP A		34.1		41.276	31.6			31.36
	ATOM	2618	СВ	TRP A		35.3		43.033	34.4			30.98
	ATOM	2619	CG	TRP A		36.7		42.617	33.9		1.00	
	ATOM	2620		TRP A		37.3		43.116	32.9		1.00	22.83
45	MOTA	2621		TRP A		37.€		41.653	34.5	533	1.00	21.90
	ATOM	2622	NE1			38.6	537	42.556	32.7	764	1.00	26.63
	ATOM	2623	CE2	TRP A	353	38.8	316	41.631	33.7	743	1.00	24.09
	ATOM	2624		TRP A		37.6	523	40.821	35.6			21.95
	ATOM	2625		TRP A		39.8		40.814	34.0			23.28
50	ATOM	2626	CZ3	TRP A		38.7		39.999	35.9			18.74
-	ATOM	2627	CH2	TRP A		39.8	228	40.007	35.0			23.86
	ATOM	2628	N	VAL A								
						33.9		43.460	31.8			30.38
	ATOM	2629	CA	VAL A		33.6		43.639	30.3			30.47
	ATOM	2630	C	VAL A		34.9		44.147	29.6		1.00	
55	ATOM	2631	0	VAL A		35.4		45.236	29.9		1.00	31.50
	ATOM	2632	CB	VAL A	354	32.5	598	44.726	30.1	.18	1.00	29.56
	ATOM	2633	CG1	VAL A	354	32.3	331	44.886	28.7	20		29.31
	ATOM	2634		VAL A		31.3		44.383	30.7			29.98
	ATOM	2635	N	GLY A		35.4		43.373	28.7			30.87
60	ATOM	2636	CA	GLY A		36.6		43.739	27.9			31.04
00	ATOM	2637										
			C	GLY A		37.8		43.431	28.7			31.16
	ATOM	2638	0	GLY A		37.8		42.748	29.7			31.10
	ATOM	2639	N	ARG A		39.0		43.944	28.2			32.24
	MOTA	2640	CA	ARG A		40.2		43.653	28.8			33.32
65	MOTA	2641	С	ARG A	356	40.5	551	44.699	29.9	39	1.00	33.80
	MOTA	2642	0	ARG A	356	40.4	49	44.391	31.1			33.03
	ATOM	2643	CB	ARG A		41.3		43.602	27.7			33.33
	ATOM	2644	CG	ARG A		41.4		42.265	27.0			35.53
	ATOM	2645	CD	ARG A		42.5		42.252	25.8			36.37
70	ATOM	2646	NE	ARG A		42.5		40.937	25.1			39.23
, ,	011	~ ~ ~ ~ ~	-44	and A	330	72.7		40.33 <i>1</i>	1. د م		1.00	J J . L J

5	ATOM ATOM ATOM ATOM ATOM ATOM	2647 2648 2649 2650 2651 2652	NH2	ARG PHE PHE		42.422 42.114 42.559 40.815 40.960 39.778	40.677 41.615 39.452 45.932 47.044 47.998	23.835 22.958 23.394 29.532 30.471 30.390	1.00 37.64 1.00 36.00 1.00 37.65 1.00 34.12 1.00 35.49 1.00 35.77
10	ATOM ATOM ATOM ATOM ATOM	2653 2654 2655 2656 2657 2658	O CB CG CD1 CD2 CE1	PHE PHE PHE PHE PHE	A 357 A 357 A 357 A 357 A 357 A 357	39.651 42.269 43.459 43.800 44.184 44.885	48.933 47.761 46.902 46.605 46.330 45.800	31.179 30.192 30.485 31.799 29.460 32.082	1.00 34.97 1.00 35.85 1.00 38.15 1.00 38.33 1.00 40.95 1.00 38.68
15	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2659 2660 2661 2662 2663 2664	CE2 CZ N CA C	PHE ARG ARG ARG ARG	A 357 A 358 A 358 A 358 A 358 A 358	45.269 45.618 38.897 37.711 36.922 37.391	45.527 45.261 47.706 48.497 47.799 46.871	29.739 31.057 29.437 29.157 28.024 27.430	1.00 42.58 1.00 41.21 1.00 36.06 1.00 36.46 1.00 35.36 1.00 34.09
20	ATOM ATOM ATOM ATOM ATOM	2665 2666 2667 2668 2669	CB CG CD NE CZ	ARG A	A 358 A 358 A 358 A 358 A 358	38.115 39.145 39.180 40.420 40.844	49.913 49.958 51.309 52.050 52.594	28.726 27.558 26.811 26.994 28.135	1.00 36.17 1.00 39.77 1.00 43.70 1.00 48.95 1.00 52.79
25	ATOM ATOM ATOM ATOM	2670 2671 2672 2673	NH1	ARG	A 358 A 358 A 359	40.115 42.001 35.697 34.923	52.528 53.246 48.233 47.749	29.240 28.170 27.786 26.658	1.00 52.79 1.00 56.15 1.00 52.75 1.00 34.80 1.00 33.84
30	ATOM ATOM ATOM ATOM ATOM	2674 2675 2676 2677 2678	C O CB CG CD	PRO	359 359 359 359	35.692 36.257 33.701 33.538 34.950	47.972 49.023 48.654 48.976 49.197	25.354 25.165 26.688 28.143 28.616	1.00 33.44 1.00 32.66 1.00 34.51 1.00 35.09 1.00 34.39
35	ATOM ATOM ATOM ATOM ATOM	2679 2680 2681 2682 2683	N CA C O CB	SER A SER A SER A SER A	360 360 360	35.667 36.344 35.705 34.533 36.335	46.992 47.084 48.140 48.475 45.724	24.461 23.212 22.314 22.423 22.527	1.00 31.83 1.00 30.20 1.00 29.79 1.00 29.04 1.00 30.82
40	ATOM ATOM ATOM ATOM ATOM	2684 2685 2686 2687 2688	OG N CA C	SER AGLU AGLU AGLU AGLU A	360 361 361 361	35.019 36.525 36.077 35.319 35.743	45.301 48.701 49.715 49.111 48.116	22.235 21.450 20.532 19.332 18.782	1.00 29.59 1.00 29.11 1.00 30.22 1.00 29.39 1.00 27.57
45	ATOM ATOM ATOM ATOM ATOM	2689 2690 2691 2692 2693	CB CG CD	GLU A GLU A GLU A	361 361 361 361	37.312 37.141 38.464 39.487 38.490	50.426 51.253 51.764 51.227 52.699	20.028 18.799 18.297 18.751 17.475	1.00 30.69 1.00 34.45 1.00 38.00 1.00 44.33 1.00 40.62
50	ATOM ATOM ATOM ATOM ATOM	2694 2695 2696 2697 2698	N CA C O CB	PRO A PRO A PRO A PRO A	362 362 362 362	34.228 33.482 34.118 34.522 32.160	49.754 49.427 50.047 51.189 50.116	18.941 17.716 16.461 16.533 17.938	1.00 40.62 1.00 30.05 1.00 30.28 1.00 30.65 1.00 30.95 1.00 30.19
55	ATOM ATOM ATOM ATOM ATOM	2699 2700 2701 2702 2703	CG CD N CA C	PRO A PRO A HIS A HIS A	362 363 363 363	32.417 33.630 34.185 34.766 33.636	51.216 50.892 49.309 49.766 49.717	18.892 19.653 15.348 14.099 13.044	1.00 29.85 1.00 30.30 1.00 30.69 1.00 31.18 1.00 32.07
60	ATOM ATOM ATOM ATOM ATOM	2704 2705 2706 2707 2708		HIS A HIS A HIS A HIS A	363 363 363	33.249 35.898 37.104 37.120 38.313	48.637 48.828 48.970 48.604 49.509	12.585 13.709 14.572 15.905 14.316	1.00 32.01 1.00 31.43 1.00 30.92 1.00 33.58 1.00 31.13
65	ATOM ATOM ATOM ATOM ATOM	2709 2710 2711 2712 2713	CE1 NE2 N CA C	HIS A HIS A PHE A PHE A PHE A	363 363 364 364 364	38.309 39.052 33.116 31.934 32.243	48.864 49.412 50.892 51.036 50.969	16.413 15.467 12.705 11.883 10.422	1.00 32.05 1.00 33.31 1.00 31.92 1.00 32.06 1.00 32.54
70	ATOM ATOM ATOM	2714 2715 2716	СВ	PHE A PHE A PHE A	364	33.218 31.233 30.437	51.536 52.387 52.437	9.961 12.149 13.439	1.00 31.64 1.00 31.72 1.00 31.78

		0545				264	00 000	FO 110	12 464	1 00	27.81
	ATOM	2717		PHE			29.090	52.119	13.464		
	ATOM	2718		PHE			31.053	52.790	14.639		33.24
	ATOM	2719		PHE			28.378	52.176	14.613		29.56
_	ATOM	2720		PHE			30.352	52.821	15.795 15.784		31.13 32.61
5	ATOM	2721	CZ	PHE			28.986	52.518 50.293	9.674		33.31
	ATOM	2722	N	THR			31.368		8.253		34.57
	ATOM	2723	CA	THR			31.498	50.288	7.819		34.99
	ATOM	2724	C	THR			31.228 30.651	51.716 52.496	8.546		34.77
10	ATOM	2725	O	THR			30.504	49.317	7.601		35.03
10	ATOM	2726	CB	THR THR			29.176	49.517	8.001		38.45
	ATOM	2727		THR			30.681	47.938	8.127		34.53
	ATOM	2728		LEU			31.672	52.053	6.623		36.44
	ATOM	2729	N				31.561	53.401	6.106		37.06
15	ATOM	2730	CA	LEU			30.167	53.401	6.119		37.17
15	ATOM	2731	C	LEU			30.107	55.214	6.280		37.82
	ATOM	2732	O	LEU			30.032	53.415	4.667		37.55
	ATOM	2733	CB	LEU			33.483	53.415	4.390		39.89
	ATOM	2734 2735	CG CD1	LEU LEU			33.403	54.070	2.878		41.97
20	ATOM	2736	-	LEU			33.776	55.209	5.134		42.04
20	ATOM ATOM	2737	N N	ASP			29.139	53.174	5.912		36.03
	ATOM	2738	CA	ASP			27.773	53.701	5.888		36.01
	ATOM	2739	CA	ASP			27.199	53.701	7.269		34.74
	ATOM	2740	ŏ	ASP			26.175	54.561	7.426		34.21
25	ATOM	2741	CB	ASP			26.812	52.825	5.054		36.66
23	ATOM	2742	CG	ASP			26.868	51.345	5.410		38.11
	ATOM	2742		ASP			27.230	50.976	6.536		38.62
	ATOM	2744		ASP			26.578	50.456	4.579		43.47
	ATOM	2745	N N	GLY			27.856	53.316	8.258		33.46
30	ATOM	2746	CA	GLY	-	·	27.506	53.488	9.650,		32.51
30	ATOM	2747	C	GLY			26.426	52.599	10.153		31.58
	ATOM	2748	Ö	GLY			25.992	52.784	11.281		30.96
	ATOM	2749	N	ASN			25.998	51.633	9.334		30.28
	ATOM	2750	CA	ASN			24.828	50.848	9.660		29.27
35	ATOM	2751	C	ASN			25.249	49.571	10.281		28.67
55	ATOM	2752	ŏ	ASN			24.417	48.759	10.684		28.60
	ATOM	2753	ČВ	ASN			24.027	50.569	8.372		30.29
	ATOM	2754	CG	ASN			23.406	51.857	7.752		29.97
	ATOM	2755	-	ASN			23.046	52.775	8.459	1.00	30.57
40	ATOM	2756		ASN			23.263	51.880	6.433		31.70
	ATOM	2757	N	SER			26.561	49.372	10.370		27.14
	ATOM	2758	CA	SER			27.082	48.168	10.954	1.00	26.22
	ATOM	2759	С	SER			28.511	48.399	11.463	1.00	25.28
	ATOM	2760	0	SER	A 3	370	29.195	49.343	11.038	1.00	21.89
45	ATOM	2761	CB	SER			27.082	47.027	9.927	1.00	25.88
	ATOM	2762	OG	SER	A 3	370	27.952	47.340	8.858	1.00	30.29
	ATOM	2763	N	PHE			28.929	47.505	12.362		25.10
	ATOM	2764	CA	PHE	A 3	371	30.242	47.615			26.36
	ATOM	2765	С	PHE			30.828	46.295	13.463		25.97
50	ATOM	2766	0	PHE			30.118	45.320	13.638		26.84
	ATOM	2767	CB	PHE			30.188	48.599	14.177		26.14
	MOTA	2768	CG	PHE			29.275	48.201	15.265		27.08
	ATOM	2769		PHE			29.715	47.412	16.300		30.96
	ATOM	2770		PHE			27.974	48.642	15.299		25.40
55	ATOM	2771		PHE			28.856	47.055	17.334		26.99
	ATOM	2772		PHE	A 3	371	27.148	48.280	16.324		24.25
	ATOM	2773	CZ	PHE			27.586	47.490	17.320		26.85
	ATOM	2774	N	TYR			32.139	46.271	13.632		26.28
	ATOM	2775	CA	TYR			32.825	45.074	14.091		26.83
60	ATOM	2776	C	TYR			33.463	45.428	15.431		28.08
	ATOM	2777	0	TYR	A 3	372	33.841	46.570	15.649		28.37
	ATOM	2778	CB	TYR			33.879	44.638	13.069		26.10
	ATOM	2779	CG	TYR			33.347	44.403	11.661		26.71
·-	ATOM	2780		TYR			33.028	45.443	10.832		26.09
65	MOTA	2781	CD2	TYR	A 3	3/2	33.209	43.138	11.160		29.23
	ATOM	2782		TYR			32.556	45.227	9.569		26.18
	MOTA	2783	CE2				32.743	42.916	9.900		28.68
	MOTA	2784	CZ	TYR			32.424	43.958	9.117		27.90
70	MOTA	2785	ОН	TYR	A) / <u>/</u>	31.973	43.707	7.864		31.58
70	ATOM	2786	N	LYS	A S	3/3	33.613	44.443	16.313	I.00	28.86

	ATOM	278	7 CA	LYS	A 373	34.072	2 44.70	7 17.65	5 1.00 29.30
	ATOM		_	LYS	A 373	34.489	9 43.36		
	ATOM ATOM				A 373 A 373	33.875 32.880			
:	5 атом	279	1 CG	LYS	A 373	32.978			
	ATOM ATOM				A 373	31.682	46.194	20.346	1.00 32.41
	ATOM				A 373 A 373	31.844 32.598			
	ATOM	2795	5 N		A 374	35.499			
10	MOTA (ATOM				A 374	36.021	42.191	19.781	1.00 29.20
	ATOM		_		A 374 A 374	35.148 34.898			
	ATOM	2799) CB	ILE	A 374	37.494			
15	MOTA 6	2800 2801		ILE	A 374	38.384	42.477	18.987	1.00 32.01
1.5	ATOM	2802		ILE	A 374 A 374	37.993 39.681			
	ATOM	2803	N		A 375	34.706	40.641		
	ATOM ATOM	2804 2805	-		A 375	33.741	40.154	22.089	1.00 28.41
20		2806			A 375 A 375	34.173 34.505			
	ATOM	2807	CB	ILE A	A 375	32.327		21.650 21.440	1.00 26.80 1.00 28.32
	MOTA MOTA	2808 2809		ILE A	A 375	31.805	41.337	20.929	1.00 30.15
	ATOM	2810	CD1		A 375 A 375	31.333 31.377	39.397 42.302	22.409	1.00 29.72
25	ATOM	2811	N	SER A	A 376	34.147	38.492	21.983 23.784	1.00 30.99 1.00 27.89
	ATOM ATOM	2812 2813			A 376	34.455	37.167	24.279	1.00 29.16
	ATOM	2814	C O		A 376 A 376	33.410 32.236	36.201 36.458	23.729 23.875	1.00 30.08
20	ATOM	2815	CB	SER A	A 376	34.383	37.165	25.822	1.00 29.10 .1.00 29.45
30	ATOM ATOM	2816 2817			A 376	34.900	35.961	26.326	1.00 31.37
	ATOM	2818	CA	ASN A		33.814 32.823	35.100 34.179	23.102 22.567	1.00 31.00 1.00 32.06
	ATOM	2819	C	ASN A	377	32.376	33.201	23.630	1.00 32.06
35	ATOM ATOM	2820 2821		ASN A		32.726	33.353	24.800	1.00 34.39
	ATOM	2822		ASN A		33.288 34.414	33.481 32.523	21.302 21.538	1.00 32.07 1.00 30.43
	ATOM	2823		ASN A		35.098	32.122	20.596	1.00 30.43
	ATOM ATOM	2824 2825		ASN A		34.622	32.151	22.767	1.00 28.95
40	ATOM	2826		GLU A		31.595 30.991	32.205 31.306	23.245 24.233	1.00 35.46 1.00 37.20
	ATOM ATOM	2827		GLU A		32.021	30.328	24.877	1.00 37.20
	ATOM	2828 2829		GLU A GLU A		31.752 29.697	29.722 30.690	25.896	1.00 37.33
	ATOM	2830		GLU A		29.425	29.208	23.617 23.836	1.00 37.64 1.00 43.49
45	ATOM ATOM	2831		GLU A		28.157	28.707	23.103	1.00 49.09
	ATOM	2832 2833		GLU A GLU A		27.131 28.168	29.431 27.584	23.082	1.00 54.01
	MOTA	2834		GLU A		33.225	30.231	22.544 24.340	1.00 53.42 1.00 35.87
50	ATOM ATOM	2835		GLU A		34.270	29.437	24.982	1.00 36.04
50	ATOM	2836 2837		GLU A GLU A		35.201 36.183	30.351 29.909	25.781	1.00 34.45
	ATOM	2838	CB (GLU A	379	35.131	28.688	26.363 23.957	1.00 34.05 1.00 37.56
	ATOM ATOM	2839 2840	CG (GLU A GLU A	379	34.483	27.505	23.249	1.00 41.83
55	ATOM	2841	OE1	GLU A	379 379	33.709 34.052	27.905 28.946	22.009 21.394	1.00 48.27
	ATOM	2842	OE2 (GLU A	379	32.738	27.172	21.652	1.00 50.70 1.00 53.49
	ATOM ATOM	2843 2844		GLY A		34.922	31.634	25.802	1.00 32.96
	ATOM	2845		GLY A		35.759 36.963	32.536 33.130	26.570	1.00 32.06
60	ATOM	2846	0 0	LY A	380	37.865	33.130	25.827 26.488	1.00 30.76 1.00 30.06
	ATOM ATOM	2847 2848		YR A		36.942	33.106	24.490	1.00 29.35
	ATOM	2849		YR A		37.990 37.496	33.659 34.879	23.635	1.00 29.39
/-	MOTA	2850	r o	YR A	381	36.388	34.879	22.840 22.230	1.00 28.64 1.00 28.59
65	ATOM ATOM	2851 2852		YR A		38.602	32.594	22.691	1.00 30.01
	ATOM	2853	CD1 T	YR A		39.328 38.625	31.479 30.401	23.441 23.962	1.00 31.34
	MOTA	2854	CD2 T	YR A	381	40.698	31.535	23.902	1.00 34.09 1.00 31.70
70	ATOM ATOM	2855 2856	CE1 T	YR A	381	39:258	29.401	24.666	1.00 32.67
. •		2000	CEZ T	и А	201	41.338	30.526	24.368	1.00 29.86

	ATOM ATOM	2857 2858	CZ OH			381 381	40.604 41.210	29.474 28.462	24.862 25.564	1.00	32.07 36.44
	ATOM	2859	N			382	38.341	35.900	22.839		27.18
	ATOM	2860	CA			382	38.030	37.190	22.262		27.54
5	ATOM	2861	С	ARG	Α	382	38.183	37.171	20.751	1.00	27.17
	MOTA	2862	0			382	39.281	37.077	20.241	1.00	27.99
	MOTA	2863	CB			382	38.916	38.274	22.890		27.41
	MOTA	2864	CG			382	38.377	38.750	24.239	1.00	
	ATOM	2865	CD			382	39.355	39.449	25.210		28.40
10	ATOM	2866	NE			382	38.855	39.054	26.526		27.90
	MOTA	2867	CZ			382	37.797	39.602	27.121	1.00	25.68
	ATOM ATOM	2868 2869		ARG ARG			37.165	40.666	26.618 28.224		27.00
	ATOM	2870	NAZ N			383	37.370 37.064	39.080 37.313	28.224		24.84 26.95
15	ATOM	2871	CA			383	37.004	37.313	18.595		25.86
13	ATOM	2872	C			383	36.196	38.388	18.029		26.13
	ATOM	2873	ŏ			383	35.551	39.124	18.766		26.39
	ATOM	2874	ČВ			383	36.436	35.902	18.170		25.61
	ATOM	2875	CG	HIS	Α	383	37.439	34.812	18.260		25.70
20	ATOM	2876	ND1	HIS	Α	383	38.503	34.733	17.391	1.00	23.67
	MOTA	2877		HIS			37.604	33.812	19.161		23.59
	ATOM	2878		HIS			39.282	33.728	17.761		22.66
	ATOM	2879		HIS			38.773	33.173	18.845		19.46
25	ATOM	2880	N			384	36.232	38.547	16.715		25.92
23	ATOM ATOM	2881 2882	CA C			384 384	35.586 34.165	39.671 39.283	16.091 15.784	1.00	
	ATOM	2883	Ö			384	33.921	38.262	15.764	1.00	
	ATOM	2884	СВ			384	36.306	40.039	14.778	1.00	
	ATOM	2885		ILE			37.734	40.458	15.054		27.00
30	ATOM	2886		ILE			35.552	41.135	14.042		26.58
	ATOM	2887	CD1	ILE	Α	384	38.700	40.235	13.849		29.40
	ATOM	2888	N	CYS	Α	385	33.238	40.114	16.222	1.00	27.67
	MOTA	2889	CA			385	31.854	39.885	15.968		28.87
25	ATOM	2890	Ċ			385	31.428	41.007	15.069		27.76
35	ATOM	2891	O	CYS			31.951	42.109	15.186		27.14
	ATOM ATOM	2892 2893	CB SG	CYS			31.028 29.828	39.905	17.272		29.48
	ATOM	2894	N N	CYS		386	30.466	38.587 40.709	17.270 14.189		37.72 27.09
	ATOM	2895	CA	TYR			29.895	41.657	13.260		27.30
40	ATOM	2896	C	TYR			28.467	41.893	13.698		27.66
	ATOM	2897	Ō	TYR			27.728	40.921	13.954		29.00
	ATOM	2898	CB	TYR	Α	386	29.936	41.065	11.870	1.00	27.12
	MOTA	2899	CG	TYR			29.181	41.792	10.797		26.46
	ATOM	2900	CD1				29.530	43.057	10.410		22.92
45	ATOM	2901		TYR		386	28.133	41.158	10.124	1.00	27.21
	ATOM ATOM	2902 2903		TYR TYR			28.844 27.428	43.692	9.400		26.58 27.27
	ATOM	2903	CEZ			386	27.428 27.788	41.801 43.055	9.142 8.773		26.83
	ATOM	2905	OH	TYR			27.075	43.689	7.788		29.03
50	ATOM	2906	N	PHE			28.110	43.172	13.812		27.27
	ATOM	2907	CA	PHE			26.840	43.648	14.343		27.38
	ATOM	2908	С	PHE	Α	387	26.159	44.523	13.298		27.63
	ATOM	2909	0	PHE	Α	387	26.830	45.404	12.719	1.00	27.68
	MOTA	2910	СВ	PHE			27.100	44.625	15.526		27.34
55	MOTA	2911	CG	PHE			27.511	43.969	16.806		28.85
	MOTA	2912		PHE			28.871	43.725	17.092		31.74
	MOTA	2913		PHE			26.575	43.626	17.750		28.35
	ATOM ATOM	2914 2915		PHE PHE			29.245	43.137	18.294		29.31
60	ATOM	2915	CEZ	PHE			26.965 28.294	43.056 42.800	18.952 19.210		30.57 30.81
00	MOTA	2917	N	GLN			24.852	44.352	13.101		27.28
	ATOM	2918	CA	GLN			24.102	45.249	12.225		28.29
	ATOM	2919	C.	GLN			23.250	46.113	13.095		28.91
	ATOM	2920	ŏ	GLN			22.579	45.663	13.993		29.61
65	MOTA	2921	СВ	GLN			23.320	44.493	11.152		27.95
	MOTA	2922	CG	GLN			24.261	43.652	10.242		29.84
	MOTA	2923	CD	GLN			23.520	42.916	9.116		30.76
	ATOM	2924		GLN			22.495	42.320	9.359		32.29
70	ATOM	2925		GLN			24.056	42.966	7.896		32.24
70	MOTA	2926	N	ILE	Α	389	23.244	47.385	12.822	1.00	31.80

5	ATOM ATOM ATOM ATOM ATOM ATOM	2928 2929 2930 2931	CB CB CB	ILE ILE ILE 1 ILE	A 389 A 389 A 389 A 389 A 389 A 389		22.690 21.329 21.186 22.894 24.267 21.840	48.154 48.523 49.752 50.161	14.439 15.619 13.337 13.838	1.00 36.24 1.00 39.05 1.00 34.30 1.00 35.49
10	ATOM ATOM	2933 2934 2935 2936 2937 2938	CD N CA C C C C	1 ILE ASP ASP ASP ASP ASP	A 389 A 390 A 390 A 390 A 390 A 390		24.667 20.342 19.049 18.648 17.470 17.920	51.476 47.603 47.422 45.969 45.665 48.129	13.397 13.764 14.446 14.536 14.668	1.00 37.16 1.00 37.12 1.00 38.19 1.00 37.79
15	ATOM ATOM	2939 2940 2941 2942 2943	OD: OD: N CA	1 ASP 2 ASP LYS LYS	A 390 A 391 A 391		17.817 17.580 17.971 19.622 19.362	49.835 50.513 45.083 43.655		1.00 41.07 1.00 45.39 1.00 43.05 1.00 36.90 1.00 36.88
20	ATOM ATOM ATOM ATOM ATOM	2944 2945 2946 2947 2948	Ō	LYS LYS LYS	A 391 A 391 A 391 A 391 A 391		19.915 20.926 20.103 19.262 20.093	43.078 43.539 43.015 42.731 41.805	15.622 16.121 13.160 11.901 10.904	1.00 35.55 1.00 33.43 1.00 37.29 1.00 41.18 1.00 45.70
25	ATOM ATOM ATOM ATOM ATOM	2949 2950 2951 2952 2953	CE NZ N CA C	LYS L LYS L LYS L	A 391 A 391 A 392 A 392 A 392		19.397 20.375 19.278 19.758 21.064	41.478 41.390 42.036 41.339	9.550 8.330 16.103 17.270	1.00 45.90 1.00 46.25 1.00 35.58 1.00 36.06
30	ATOM ATOM ATOM ATOM ATOM	2954 2955 2956 2957 2958	O CB CG CD CE	LYS A LYS A LYS A	A 392 A 392 A 392 A 392		21.482 18.722 18.442 17.712	40.596 40.424 40.300 39.262 38.042	17.002 15.839 17.661 16.551 17.122	1.00 36.18 1.00 35.91 1.00 36.65 1.00 38.84 1.00 41.45
35	ATOM ATOM ATOM	2959 2960 2961 2962	NZ N CA C	LYS A LYS A ASP A ASP A	A 392 A 393 A 393 A 393	٠	16.893 16.224 21.667 22.823 23.968	37.290 36.066 40.138 39.268 39.817	16.095 16.691 18.099 18.103 17.239	1.00 41.02 1.00 38.35 1.00 35.78 1.00 35.76 1.00 34.85
40	ATOM ATOM ATOM ATOM ATOM ATOM	2963 2964 2965 2966 2967 2968	OD2	ASP	393 393 393 393		23.914 22.446 21.231 21.026 20.435	40.946 37.857 37.219 37.404 36.460	16.741 17.584 18.295 19.531 17.672	1.00 33.92 1.00 36.56 1.00 40.35 1.00 42.98 1.00 42.96
45	ATOM ATOM ATOM ATOM	2969 2970 2971 2972	N CA C O CB	CYS A CYS A CYS A CYS A	394 394 394 394		25.019 26.088 26.580 26.256 27.238	39.019 39.369 38.083 36.967 40.084	17.088 16.187 15.570 16.039 16.914	1.00 33.41 1.00 33.82 1.00 32.97 1.00 32.97 1.00 34.46
50	ATOM ATOM ATOM ATOM ATOM	2973 2974 2975 2976 2977	SG N CA C	CYS A THR A THR A THR A	395 395 395 395		28.009 27.388 27.928 29.434 30.128	39.022 38.231 37.081 37.066 38.006	13.851 14.088 13.729	1.00 38.67 1.00 30.95 1.00 29.51 1.00 28.32 1.00 26.38
55	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2978 2979 2980 2981 2982 2983	CB OG1 CG2 N CA C	THR A THR A THR A PHE A PHE A PHE A	395 395 396 396		27.676 26.271 28.140 29.935 31.356 32.016	37.235 37.381 36.013 36.000 35.805 35.496	12.342 12.063 11.558 14.682 14.830	1.00 30.00 1.00 30.37 1.00 28.82 1.00 27.62 1.00 27.77
60	ATOM ATOM ATOM ATOM ATOM	2984 2985 2986 2987 2988	O CB CG CD1	PHE A PHE A PHE A	396 396 396 396		31.582 31.601 31.567 32.505	34.611 34.686 35.149 36.041	13.486 12.753 15.818 17.238 17.691	1.00 28.57 1.00 29.01 1.00 27.37 1.00 28.76 1.00 27.09
65	ATOM ATOM ATOM ATOM ATOM	2989 2990 2991 2992 2993	CE1 CE2 CZ N	PHE A PHE A PHE A ILE A ILE A	396 396 396 397		30.540 32.475 30.488 31.451 33.018	34.760 36.506 35.228 36.112 36.271	18.091 19.012 19.392 19.855 13.127	1.00 29.92 1.00 30.67 1.00 30.26 1.00 31.58 1.00 29.00
70	ATOM ATOM ATOM	2994 2995 2996	C 0	ILE A ILE A ILE A	397 397		33.729 35.123 35.741 33.821	36.054 35.411 34.942 37.354	11.878 12.098 11.151 11.057	1.00 29.41 1.00 29.48 1.00 29.78 1.00 29.93

	ATOM ATOM	2997 2998	CG2		397		34.591 32.457	38.407 37.835	11.809 10.718	1.00	29.25 29.75
	ATOM	2999	CD1				35.269	39.402	10.924	1.00	31.20
_	ATOM	3000	N	THR A			35.589	35.367	13.339	1.00	29.02
5	ATOM ATOM	3001 3002	CA C	THR A			36.754 36.380	34.565 33.686	13.695 14.866	$1.00 \\ 1.00$	
	ATOM	3002	Ö	THR A			35.436	33.977	15.590	1.00	29.46
	ATOM	3004	СВ	THR A			37.963	35.412	14.114	1.00	29.68
	ATOM	3005		THR A			37.645	36.178	15.304	1.00	
10	ATOM	3006	CG2				38.339	36.415	13.020	1.00	
	ATOM	3007	N	LYS A	399		37.143	32.629	15.074	1.00	30.35
	ATOM	3008	CA	LYS A	399	;	36.885	31.683	16.156	1.00	32.18
	MOTA	3009	С	LYS A			38.149	30.867	16.321		30.94
	ATOM	3010	0	LYS A			38.960	30.812	15.422		30.64
15	ATOM	3011	CB	LYS A			35.741	30.716	15.802		33.03
	ATOM	3012	CG	LYS A			34.969	31.118	14.547		39.43
	MOTA MOTA	3013 3014	CD	LYS A LYS A			33.751 32.554	30.221 31.100	14.171 13.683		44.29 45.24
	ATOM	3014	NZ	LYS A			31.425	30.316	13.063		48.22
20	ATOM	3016	N	GLY A			38.297	30.231	17.468		30.34
20	ATOM	3017	CA	GLY A			39.430	29.389	17.734		30.41
	ATOM	3018	C	GLY A			39.998	29.650	19.130	1.00	31.49
	ATOM	3019	0	GLY A	400		39.655	30.639	19.811	1.00	29.63
	ATOM	3020	N	THR A	401	4	40.858	28.738	19.558	1.00	
25	ATOM	3021	CA	THR A			41.543	28.879	20.828		34.07
	ATOM	3022	C	THR A			12.763	29.832	20.740		32.71
	ATOM	3023	0_	THR A			43.892	29.401	20.778		34.00
	ATOM	3024	CB	THR A			11.978	27.494	21.314		34.50
30	ATOM ATOM	3025 3026	OG1 CG2				10.812 12.610	26.676 27.608	21.574 22.641		39.26 36.18
50	ATOM	3027	N	TRP A			12.508	31.126	20.642	1.00	
	ATOM	3028	CA	TRP A			13.548	32.138	20.576	1.00	
	ATOM	3029	C	TRP A			12.723	33.392	20.565	1.00	
	ATOM	3030	0	TRP A	402		11.507	33.307	20.544	1.00	25.60
35	ATOM	3031	CB	TRP A			14.383	32.037	19.298		28.72
	ATOM	3032	CG	TRP A			13.607	31.774	18.069		29.95
	MOTA	3033		TRP A			13.274	30.538	17.553		31.24
	ATOM ATOM	3034 3035	NE1	TRP A			13.058 12.541	32.735 30.686	17.160 16.405		30.14 29.78
40	ATOM	3036	CE2				12.397	32.017	16.133		30.91
	ATOM	3037	CE3	TRP A			13.042	34.122	17.113		30.21
	ATOM	3038		TRP A			11.723	32.643	15.094		30.88
	MOTA	3039	CZ3	TRP A	402		12.385	34.744	16.073		31.74
	MOTA	3040	CH2	TRP A			11.730	34.008	15.077		30.37
45	ATOM	3041	N	GLU A			13.325	34.564	20.491		27.23
	ATOM	3042	CA	GLU A			12.468	35.748	20.447		26.73
	ATOM	3043	C	GLU A			12.904	36.792	19.498		25.83 24.50
	MOTA MOTA	3044 3045	O CB	GLU A			4.103 2.383	36.972 36.461	19.227 21.830		27.45
50	ATOM	3046	CG	GLU A			2.176	35.552	23.036		28.63
•	ATOM	3047	CD	GLU A			1.798	36.314	24.299		31.80
	MOTA	3048		GLU A			2.453	37.326	24.598		30.89
	MOTA	3049	OE2	GLU A	403	4	0.842	35.882	24.992		36.19
	MOTA	3050	N	VAL A			1.899	37.558	19.077		25.24
55	MOTA	3051	CA	VAL A			2.127	38.736	18.314		24.95
	MOTA	3052	C	VAL A			2.569	39.806	19.296		26.20
	ATOM	3053	O	VAL A			11.944	39.991	20.353		25.92
	ATOM ATOM	3054 3055	CB CG1	VAL A			0.908 1.217	39.172 40.371	17.633 16.843		24.47 26.01
60	MOTA	3056		VAL A			0.379	38.055	16.711		25.01
	ATOM	3057	N	ILE A			3.646	40.501	18.960		26.33
	MOTA	3058	CA	ILE A			4.216	41.481	19.848		27.21
	ATOM	3059	C	ILE A		4	3.658	42.828	19.568		26.94
_	MOTA	3060	0	ILE A	405	4	3.341	43.569	20.467	1.00	27.10
65	MOTA	3061	CB	ILE A			5.726	41.499	19.685		28.08
	ATOM	3062		ILE A			6.290	40.270	20.389		29.19
	ATOM ATOM	3063 3064		ILE A			6.301	42.773	20.334		29.53
	ATOM	3065	N	ILE A GLY A			7.238 3.505	39.565 43.133	19.592 18.299		32.57 26.78
70	ATOM	3066	CA	GLY A			2.928	44.393	17.909		26.62
-		-				-					

5	ATOM ATOM ATOM ATOM ATOM ATOM	3067 3068 3069 3070 3071 3072	O N CA	GLY ILE ILE ILE	A 406 A 406 A 407 A 407 A 407 A 407		42.486 43.010 41.493 41.097 41.827 41.705	43.541 45.141 45.320 46.578	15.673 16.126 14.747 14.245	1.00 1.00 1.00	25.77 27.03 27.04
10	ATOM ATOM ATOM ATOM ATOM ATOM	3073 3074 3075 3076 3077 3078	CB CG: CD: N	ILE 1 ILE 2 ILE 1 ILE GLU	A 407 A 407 A 407		39.593 38.838 39.227 37.368 42.507 43.382	45.587 44.334 46.096 44.598 46.509	14.689 15.103 13.298 15.531	1.00 1.00 1.00 1.00	26.94
15	ATOM ATOM ATOM ATOM ATOM ATOM	3079 3080 3081 3082 3083 3084		GLU . GLU . GLU .	A 408 A 408 A 408 A 408 A 408 A 408		42.929 43.285 44.748 45.292 45.563 46.036	49.590 47.060 46.188 46.968	11.473 11.350 12.328 13.431 14.691	1.00 1.00 1.00 1.00	27.19 26.59 27.48 28.71 29.19
20	ATOM ATOM ATOM ATOM	3085 3086 3087 3088	OE2 N CA C	GLU A ALA A ALA	A 408 A 409 A 409 A 409		45.311 42.171 41.609 40.409	46.411	14.625 15.740 10.583 9.464 8.841	1.00	
25	ATOM ATOM ATOM ATOM ATOM	3089 3090 3091 3092 3093	O CB N CA C	ALA A LEU A LEU A	A 409 A 409 A 410 A 410 A 410		40.258 42.649 39.587 38.356	46.600 48.820 48.625 48.130	8.909 8.448 8.187 7.595	1.00 1.00 1.00	27.79 26.95 29.93 31.53
30	ATOM ATOM ATOM ATOM ATOM	3094 3095 3096 3097 3098	O CB CG CD1 CD2	LEU A LEU A LEU A	A 410 A 410 A 410 A 410		38.122 38.068 37.213 35.865 34.773 35.860	48.796 50.000 48.493 47.763 48.737 46.511	6.276 6.214 8.515 8.429 8.020 7.533	1.00 1.00 1.00 1.00	31.83 30.83 31.79 34.75 34.78 34.05
35	ATOM ATOM ATOM ATOM ATOM	3099 3100 3101 3102 3103	N CA C O CB	THR A THR A THR A THR A	411 411 411 411		38.011 37.615 36.421 36.029 38.706	48.011 48.548 47.729 46.811 48.343	5.213 3.918 3.500 4.222 2.869	1.00 1.00 1.00 1.00	33.31 34.38 34.97 34.40 34.65
40	ATOM ATOM ATOM ATOM ATOM	3104 3105 3106 3107 3108	OG1		411 411 412 412		38.923 40.014 35.905 34.772 34.877	46.934 48.894 48.016 47.309	2.726 3.335 2.299 1.697	1.00 1.00 1.00 1.00	35.94 35.71 36.01 36.64
45	ATOM ATOM ATOM ATOM ATOM	3109 3110 3111 3112 3113	O CB OG N CA	SER A SER A SER A ASP A	412 412 412 413		34.677 33.891 34.616 34.192 36.054 36.320	45.792 45.081 47.740 49.076 45.322 43.913	1.670 1.952 0.231 0.121 1.275	1.00 1.00 1.00 1.00	36.51 37.08 37.15 38.14 35.36
50	ATOM ATOM ATOM ATOM ATOM	3114 3115 3116 3117 3118	C O CB CG OD1	ASP A ASP A ASP A	413 413 413 413		37.089 37.116 37.122 36.506	43.196 41.966 43.802 44.618	1.011 2.097 2.130 -0.290 -1.427	1.00 1.00 1.00 1.00	36.07 34.65 34.82 36.80 40.03
55	ATOM ATOM ATOM ATOM ATOM	3119 3120 3121 3122 3123	OD2 N CA C	ASP A ASP A TYR A TYR A TYR A TYR A	413 414 414 414		35.273 37.176 37.740 38.603 38.612 38.589	44.524 45.405 43.946 43.310 43.975 45.206	-1.685 -2.109 2.977 3.950 5.315 5.422	1.00 1.00 1.00	42.94 43.99 33.46 32.77 30.84
60	ATOM ATOM ATOM ATOM ATOM	3124 3125 3126 3127 3128	CB CG CD1 CD2 CE1	TYR A TYR A TYR A TYR A TYR A	414 414 414 414	•	40.051 40.316 40.564 40.369 40.822	43.363 42.543 41.183 43.137 40.427	3.422 2.178 2.273 0.915 1.159	1.00 1.00 1.00 1.00	33.72 36.47 40.26 37.42
65	ATOM ATOM ATOM ATOM ATOM	3129 3130 3131 3132 3133	CE2 CZ OH N	TYR A TYR A TYR A LEU A LEU A	414 414 414 415		40.629 40.848 41.112 38.613 38.906	42.385 41.021 40.217 43.155	-0.221 -0.086 -1.184 6.351	1.00 1.00 1.00 1.00	38.74 40.96 45.05 28.44
70	ATOM ATOM ATOM	3134 3135 3136	C 0	LEU A LEU A LEU A	415 415		40.332 40.671 37.923	43.631 43.153 41.994 43.082	7.682 8.016 7.804 8.698	1.00 1.00 1.00	26.61

	A TOM	3137	CG	1 511	7	415		38.089	43.643	10.096	1 00	26.32
	ATOM ATOM	3138		LEU				36.785	43.538	10.868		26.32
	ATOM	3139		LEU				39.212	42.913	10.798		24.32
	ATOM	3140	N			416		41.169	44.047	8.541		27.81
5	ATOM	3141	CA			416		42.513	43.648	8.909		27.67
•	ATOM	3142	C	TYR				42.594	43.578	10.447		27.84
	ATOM	3143	ŏ	TYR				41.948	44.334	11.150		28.65
	ATOM	3144	ČВ	TYR				43.530	44.631	8.325		27.67
	ATOM	3145	CG	TYR				43.603	44.705	6.801		26.27
10	ATOM	3146		TYR	Α	416		42.648	45.398	6.065	1.00	24.50
	ATOM	3147		TYR				44.655	44.110	6.103	1.00	26.34
	ATOM	3148	CE1	TYR	Α	416		42.734	45.514	4.695	1.00	26.01
	ATOM	3149	CE2	TYR	Α	416		44.730	44.204	4.747	1.00	26.06
	ATOM	3150	CZ	TYR	Α	416		43.772	44.914	4.046		26.01
15	MOTA	3151	OH	TYR	A	416		43.840	44.993	2.696		34.51
	ATOM	3152	N	TYR				43.374	42.651	10.976		27.82
	MOTA	3153	CA	TYR				43.477	42.514	12.420		26.63
	ATOM	3154	C	TYR				44.745	41.820	12.866		26.21
20	ATOM	3155	0	TYR				45.447	41.191	12.063		24.79
20	ATOM	3156	CB	TYR				42.258	41.763	12.991		26.04
	MOTA	3157	CG	TYR				42.222	40.301	12.668		24.88
	ATOM	3158 3159	CD1					41.636 42.739	39.838 39.372	11.495 13.549		26.75 22.61
	ATOM	3160	CD2 CE1					42.739	38.450	11.216		25.54
25	ATOM ATOM	3161	CE2					42.728	38.056	13.274		22.53
43	ATOM	3162	CZ	TYR				42.720	37.586	12.106		23.32
	ATOM	3163	OH	TYR				42.132	36.225	11.888		20.94
	ATOM	3164	N	ILE				45.014	41.940	14.176		26.21
	ATOM	3165	CA	ILE				46.177	41.339	14.811		25.01
30	ATOM	3166	C	ILE				45.748	40.303	15.767		24.88
	ATOM	3167	ŏ	ILE				44.818	40.526	16.547		25.94
	ATOM	3168	CB	ILE				47.000	42.390	15.518	1.00	25.33
	ATOM	3169	CG1	ILE				47.674	43.234	14.470	1.00	28.85
	ATOM	3170	CG2	ILE	Α	418		48.059	41.769	16.379	1.00	24.12
35	ATOM	3171	CD1	ILE	Α	418		48.540	44.194	15.030	1.00	31.68
	MOTA	3172	N	SER				46.420	39.155	15.743		24.26
	ATOM	3173	CA	SER				46.106	38.103	16.678		25.53
	MOTA	3174	С	SER .				47.312	37.280	17.061		25.14
	ATOM	3175	0	SER				48.396	37.373	16.451		25.43
40	ATOM	3176	СВ	SER .				45.066	37.149	16.081		26.23
	ATOM	3177	OG	SER .				45.697	36.205	15.211		28.19
	ATOM	3178	N	ASN .				47.099	36.430	18.042		25.39
	MOTA	3179 3180	CA	ASN .				48.130 47.898	35.491 34.036	18.489 18.027		26.17 26.94
45	ATOM ATOM	3181	C	ASN .				48.406	33.088	18.641		27.30
43	ATOM	3182	CB	ASN .				48.376	35.601	20.035		25.12
	ATOM	3183	CG	ASN .				47.212	35.187	20.883		24.08
	ATOM	3184		ASN .				47.257		22.141		25.35
	ATOM	3185		ASN .				46.176	34.692	20.269		19.89
50	ATOM	3186	N	GLU .				47.169	33.861	16.920		28.64
	ATOM	3187	CA	GLU				46.899	32.514	16.372		29.10
	MOTA	3188	С	GLU .				48.151	31.761	15.959	1.00	29.52
	ATOM	3189	0	GLU .	A	421		48.269	30.590	16.247	1.00	29.85
	ATOM	3190	CB	GLU .	Α	421		45.980	32.604	15.141	1.00	29.42
55	MOTA	3191	CG	GLU A	A	421		45.615	31.262	14.536		29.34
	ATOM	3192	CD	GLU /	A	421		44.558	31.362	13.432		33.30
	ATOM	3193		GLU .				44.398	32.432	12.827		32.10
	ATOM	3194		GLU A				43.872	30.354	13.176		36.08
	ATOM	3195	N	TYR .				49.081	32.435	15.287		30.59
60	MOTA	3196	CA	TYR A				50.233	31.754	14.681		31.98
	ATOM	3197	C	TYR				50.999	30.846	15.642		31.87
	ATOM	3198	0	TYR .				51.506	31.287	16.655		31.13
	MOTA	3199	CB	TYR A				51.212	32.768	14.018		32.51
65	ATOM	3200	CG CD1	TYR A				52.199	32.109	13.069		35.45
65	ATOM ATOM	3201 3202		TYR Z			•	51.754 53.568	31.303 32.294	12.014 13.200		39.38 38.76
	ATOM	3202		TYR Z				52.649	30.698	11.126		40.25
	ATOM	3203		TYR A				54.476	31.674	12.306		39.86
	ATOM	3205	CZ	TYR Z				53.997	30.881	11.287		39.55
70	ATOM	3206	ОН	TYR				54.860	30.275	10.416		43.28
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5	ATOM ATOM ATOM ATOM ATOM ATOM		CA C C CB	LYS A 42 LYS A 42 LYS A 42	3 51.821 3 51.305 3 51.957 3 53.298	28.576 28.368 27.749 28.989	16.015 17.404 18.205 16.096	1.00 33.66 1.00 33.06 1.00 32.45 1.00 34.71
10	ATOM ATOM ATOM ATOM ATOM ATOM	3213 3214 3215 3216 3217 3218	CD CE NZ N CA	LYS A 42: LYS A 42: LYS A 42: LYS A 42: GLY A 42: GLY A 42: GLY A 42:	3 55.606 3 56.503 3 57.976 4 50.128 4 49.582 4 50.375	28.785 28.952 28.612 28.901 28.755	15.070 13.824 14.100 17.706	1.00 44.73 1.00 47.80 1.00 48.84 1.00 33.60 1.00 32.49
15	ATOM ATOM	3219 3220 3221 3222 3223	O N CA C	GLY A 424 MET A 425 MET A 425 MET A 425 MET A 425	51.202 52.039 51.326 51.157	30.468 31.210 32.484 33.469	21.286 19.720 20.656 21.169 20.452	1.00 31.47 1.00 31.65
20	ATOM ATOM ATOM ATOM ATOM	3224 3225 3226 3227 3228	CB CG SD CE N	MET A 425 MET A 425 MET A 425 MET A 425 PRO A 426	54.366 55.791 56.752 50.842	31.533 30.328 30.781 31.697 32.463	19.979 19.854 18.773 19.859 22.404	1.00 32.30 1.00 34.67 1.00 43.19 1.00 40.54 1.00 29.14
25	ATOM ATOM ATOM ATOM ATOM	3229 3230 3231 3232 3233	CA C O CB CG	PRO A 426 PRO A 426 PRO A 426 PRO A 426 PRO A 426	50.830 50.261 49.586	33.599 34.917 36.028 33.123 31.593	22.894 22.991 22.904 24.255 24.176	1.00 29.32 1.00 28.68 1.00 28.13 1.00 30.45 1.00 30.82
30	ATOM ATOM ATOM ATOM ATOM	3234 3235 3236 3237 3238	CD N CA C	PRO A 426 GLY A 427 GLY A 427 GLY A 427 GLY A 427	50.957 52.137 53.011 53.544	31.390 34.794 35.949 36.321 37.026	23.398 23.123 23.152 21.800	1.00 28.81 1.00 27.82 1.00 27.65 1.00 28.12
35	ATOM ATOM ATOM ATOM ATOM	3239 3240 3241 3242	N CA C O	GLY A 428 GLY A 428 GLY A 428 GLY A 428	52.964 53.351 52.211 51.126	35.779 36.140 36.992 36.931	21.718 20.729 19.374 18.856 19.420	1.00 28.43 1.00 28.74 1.00 27.66 1.00 27.88 1.00 27.92
40	ATOM ATOM ATOM ATOM ATOM	3243 3244 3245 3246 3247	N CA C O CB	ARG A 429 ARG A 429 ARG A 429 ARG A 429	51.474 51.675 52.789 51.538	37.790 38.656 38.800 38.921 40.024	17.825 17.193 15.676 15.211 17.836	1.00 28.39 1.00 28.66 1.00 27.70 1.00 28.68 1.00 28.54
45	ATOM ATOM ATOM ATOM ATOM	3248 3249 3250 3251 3252 3253	CG CD NE CZ NH1 NH2	ARG A 429 ARG A 429 ARG A 429 ARG A 429 ARG A 429 ARG A 429	51.222 50.733 50.247 49.937 50.070 49.505	39.985 41.296 41.344 42.510 43.661 42.545	19.345 19.829 21.194 21.785 21.095	1.00 33.08 1.00 35.58 1.00 36.13 1.00 39.81 1.00 35.49
50	ATOM ATOM ATOM ATOM ATOM	3254 3255 3256 3257 3258	N CA C O CB	ASN A 430 ASN A 430 ASN A 430 ASN A 430 ASN A 430	50.571 50.591 49.336 48.218 50.767	38.825 38.901 39.533 39.455 37.530	23.058 14.919 13.457 12.861 13.408	1.00 42.19 1.00 27.66 1.00 26.33 1.00 26.87 1.00 24.20
55	ATOM ATOM ATOM ATOM ATOM	3259 3260 3261 3262 3263	CG OD1	ASN A 430 ASN A 430 ASN A 430 LEU A 431 LEU A 431	52.193 53.094 52.410 49.531	37.015 37.458 36.087 40.139	12.815 12.895 12.154 13.799 11.697	1.00 26.03 1.00 25.47 1.00 24.95 1.00 21.72 1.00 26.92
60	ATOM ATOM ATOM ATOM ATOM	3264 3265 3266 3267	C O CB CG	LEU A 431 LEU A 431 LEU A 431 LEU A 431	48.466 47.802 48.509 49.072 48.429	40.816 39.813 39.063 41.867 43.221	11.003 10.100 9.391 10.113 9.893	1.00 27.27 1.00 28.47 1.00 28.34 1.00 27.86 1.00 29.78
65	ATOM ATOM ATOM ATOM	3268 3269 3270 3271 3272	CD2 N CA C	LEU A 431 LEU A 431 TYR A 432 TYR A 432 TYR A 432	48.707 46.966 46.464 45.667 44.654	43.681 43.267 39.842 39.047 39.899	8.457 10.216 10.074 9.151 8.412	1.00 29.33 1.00 30.92 1.00 28.64 1.00 28.97 1.00 28.90
70	ATOM ATOM ATOM ATOM		CB CG	TYR A 432 TYR A 432 TYR A 432 TYR A 432	44.328 44.905 45.762 46.443	40.988 37.962 36.984 37.348	8.841 9.881 10.591 11.729	1.00 29.46 1.00 29.45 1.00 28.94 1.00 31.85

	ATOM	3277	CD2	TYR	432	45.861	35.686	10.158	1.00 29.80
	ATOM	3278	CE1			47.242	36.460	12.407	1.00 30.13
	ATOM	3279	CE2			46.635	34.774	10.830	1.00 32.21
	ATOM	3280	CZ	TYR A		47.333	35.190	11.965	1.00 30.68
5	ATOM	3281	ОН	TYR A		48.103	34.332	12.656	1.00 30.32
	ATOM	3282	N	LYS A		44.128	39.334	7.325	1.00 29.50
	ATOM	3283	CA	LYS A		43.153	39.919	6.406	1.00 29.94
	ATOM	3284	C	LYS A		42.035	38.900	6.339	1.00 30.64
	ATOM	3285	ŏ	LYS A		42.328	37.729	6.168	1.00 30.63
10	ATOM	3286	ČВ	LYS A		43.728	39.833	4.984	1.00 30.60
•	ATOM	3287	CG	LYS A		43.650	40.975	4.056	1.00 30.00
	ATOM	3288	CD	LYS A		44.453	40.571	2.841	1.00 31.31
	ATOM	3289	CE	LYS A		44.114	41.333	1.587	1.00 36.03
	ATOM	3290	NZ	LYS A		44.761	40.646	0.431	1.00 35.03
15	ATOM	3291	N	ILE A		40.784	39.355	6.385	1.00 35.93
1.5	ATOM	3292	CA	ILE A		39.617	38.531	6.221	1.00 31.20
	ATOM	3293	C	ILE A		38.837	39.076	5.071	1.00 31.63
	ATOM	3294	0	ILE A		38.403	40.224	5.107	
	ATOM	3295	CB	ILE A		38.675			1.00 31.85
20	ATOM	3296	CG1				38.672	7.412	1.00 32.38
20	ATOM	3297	CG1			39.288	38.134	8.684	1.00 33.28
	ATOM	3298	CD1			37.413	37.945	7.099	1.00 33.44 1.00 35.68
	ATOM					38.482	38.485	9.933	
	ATOM	3299 3300	N CA	GLN A		38.580	38.254	4.078	1.00 32.13
25				GLN A		37.756	38.681	2.956	1.00 32.42
25	ATOM	3301	C	GLN A		36.309	38.729	3.462	1.00 31.87
	ATOM	3302	0	GLN A		35.772	37.735	3.981	1.00 31.80
	ATOM	3303	CB	GLN A		37.959	37.725	1.773	1.00 33.28
	ATOM	3304	CG	GLN A		38.283	38.438	0.474	1.00 37.80
20	ATOM	3305	CD	GLN A		38.196	37.544	-0.759	1.00 39.65
30	ATOM	3306	OE1			37.661	37.960	-1.787	1.00 43.51
	ATOM	3307	NE2	GLN A		38.731	36.352	-0.668	1.00 36.20
	ATOM	3308	N	LEU A		35.679	39.892	3.402	1.00 31.45
	ATOM	3309	CA	LEU A		34.322	40.019	3.951	1.00 32.16
25	ATOM	3310	C	LEU A		33.214	39.216	3.211	1.00 33.57
35	ATOM	3311	0	LEU A		32.222	38.810	3.835	1.00 32.78
	ATOM	3312	CB	LEU A		33.967	41.505	4.095	1.00 32.40
	ATOM	3313	CG	LEU A		34.958	42.257	5.046	1.00 31.40
	ATOM	3314		LEU A		34.666	43.711	5.103	1.00 33.04
40	ATOM	3315		LEU A		34.920	41.684	6.449	1.00 30.51
40	ATOM	3316	N	SER A		33.418	38.892	1.938	1.00 34.25
	ATOM	3317	CA	SER A		32.403	38.123	1.202	1.00 36.72
	MOTA	3318	C	SER A		32.508	36.603	1.433	1.00 36.62
	ATOM	3319	0	SER A		31.851	35.815	0.739	1.00 40.69
	MOTA	3320	CB	SER A		32.516	38.418	-0.282	1.00 36.83
45	ATOM	3321	OG	SER A		33.806	38.070	-0.709	1.00 38.78
	ATOM	3322	N		438	33.393	36.215	2.363	1.00 35.66
	ATOM	3323	CA	ASP A		33.577	34.814	2.806	1.00 34.84
	ATOM	3324	С	ASP A		34.562	34.703	3.979	1.00 33.83
	ATOM	3325	0	ASP A		35.765	34.547	3.790	1.00 33.54
50	ATOM	3326	CB	ASP A		34.101	33.920	1.684	1.00 34.29
	ATOM	3327	CG	ASP A		34.300	32.480	2.139	1.00 33.79
	ATOM	3328		ASP A		34.227	32.222	3.362	1.00 31.81
	MOTA	3329	OD2	ASP A		34.513	31.535	1.354	1.00 32.29
	MOTA	3330	N	TYR A		34.037	34.660	5.183	1.00 33.43
55	ATOM	3331	CA	TYR A		34.867	34.735	6.372	1.00 33.14
	ATOM	3332	С	TYR A		35.881	33.611	6.504	1.00 33.75
	ATOM	3333.	0	TYR A		36.804	33.712	7.322	1.00 32.43
	MOTA	3334	CB	TYR A	439	34.009	34.815	7.618	1.00 32.78
	MOTA	3335	CG	TYR A	439	33.032	35.953	7.614	1.00 31.50
60	ATOM	3336	CD1	TYR A	439	33.363	37.196	7.084	1.00 29.56
	ATOM	3337	CD2	TYR A		31.763	35.773	8.127	1.00 31.06
	ATOM	3338	CE1	TYR A	439	32.453	38.222	7.081	1.00 32.55
	ATOM	3339	CE2	TYR A		30.846	36.776	8.107	1.00 32.77
	ATOM	3340	CZ	TYR A		31.177	37.994	7.622	1.00 32.72
65	ATOM	3341	ОН	TYR A		30.215	38.969	7.671	1.00 34.45
	ATOM	3342	N	THR A		35.743	32.555	5.705	1.00 33.09
	ATOM	3343	CA	THR A		36.749	31.515	5.737	1.00 33.93
	ATOM	3344	C	THR A		38.011	31.959	5.002	1.00 33.99
	MOTA	3345	ō	THR A		39.049	31.357	5.164	1.00 34.35
70	ATOM	3346	ČВ	THR A		36.222	30.188	5.140	1.00 34.79
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	ATOM ATOM ATOM ATOM ATOM ATOM	3348 3349 3350 3351 3352	B CG2 D N D CA L C	THR LYS LYS LYS	A 440 A 441 A 441 A 441 A 441		35.854 34.914 37.949 39.163 39.982	4 29.733 9 32.994 1 33.419 2 34.419	5.808 4.167 3.485 4.316	3 1.00 35.92 7 1.00 34.58 6 1.00 34.94 6 1.00 34.57
10	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	3354 3355 3356	CG CD CE NZ N	LYS LYS LYS LYS VAL	A 441 A 441 A 441 A 441 A 441 A 442 A 442		38.843 38.246 37.943 37.790 37.079 40.918	33.969 32.904 33.414 32.241 32.642 33.844	2.099 1.199 -0.196 -1.204 -2.444 5.081	1.00 36.12 1.00 38.45 1.00 42.38 1.00 44.53 1.00 44.38 1.00 34.16
15	ATOM	3360 3361 3362 3363 3364	C O CB CG1	VAL VAL VAL	A 442 A 442 A 442 A 442 A 442 A 442		41.807 43.264 43.788 41.744 42.371	34.386 33.300 33.883 34.805	5.623 5.575 7.405 8.445	1.00 34.50 1.00 34.09 1.00 34.66 1.00 36.89
20	ATOM	3365 3366 3367 3368 3369	N CA C O	THR THR THR THR	A 443 A 443 A 443 A 443		40.351 43.922 45.312 46.177 45.870	35.486 35.425 35.999 37.053	7.809 5.338 4.983 6.132 6.659	1.00 34.30 1.00 34.85 1.00 34.39 1.00 33.87
25	ATOM ATOM ATOM ATOM	3370 3371 3372 3373	CB OG1 CG2 N CA	THR CYS CYS	A 443 A 443 A 443 A 444 A 444		45.543 44.628 46.839 47.238 48.191	35.922	3.734 2.700 3.151 6.515 7.424	1.00 34.69 1.00 36.35 1.00 37.11 1.00 33.85 1.00 33.80
30	ATOM ATOM ATOM ATOM	3374 3375 3376 3377 3378	C O CB SG N	CYS Z CYS Z LEU Z	A 444 A 444 A 444 A 445		49.197 49.896 48.932 49.930 49.259	36.741 36.202 34.893 35.769 38.049	6.612 5.763 8.256 9.498 6.846	1.00 32.96 1.00 33.20 1.00 34.01 1.00 35.63 1.00 31.35
35	ATOM ATOM ATOM ATOM ATOM	3379 3380 3381 3382 3383	CA C O CB CG	LEU A LEU A LEU A LEU A	445 445 445 445		50.115 51.540 52.381 49.511 48.082	38.930 39.101 39.600 40.320 40.371	6.035 6.506 5.755 5.989 5.441	1.00 30.34 1.00 29.68 1.00 29.03 1.00 30.44 1.00 31.52
40	ATOM ATOM ATOM ATOM ATOM	3384 3385 3386 3387 3388	CD2 N CA	LEU A LEU A SER A SER A SER A	445 446 446		47.519 48.031 51.809 53.115 53.814	41.766 39.979 38.716 38.914 37.628	5.595 3.970 7.751 8.335 8.738	1.00 31.49 1.00 30.01 1.00 28.93 1.00 28.62 1.00 29.11
45	ATOM ATOM ATOM ATOM ATOM	3389 3390 3391 3392 3393	CB OG N	SER A SER A SER A CYS A CYS A	446 446 447		55.032 53.001 52.252 53.042 53.536	37.622 39.829 39.228 36.569 35.330	8.909 9.553 10.616 8.909	1.00 29.02 1.00 27.81 1.00 24.74 1.00 29.85
50	ATOM ATOM ATOM ATOM ATOM	3394 3395 3396 3397 3398	C O CB SG	CYS A CYS A CYS A CYS A CYS A	447 447 447 447		54.827 55.682 52.484 51.032 54.940	34.834 34.357 34.203 34.431 34.924	9.492 8.884 9.614 9.376 10.472 7.556	1.00 32.67 1.00 33.54 1.00 33.36 1.00 33.28 1.00 40.47 1.00 34.86
55	ATOM ATOM ATOM ATOM ATOM	3399 3400 3401 3402 3403	C (CB (CB (CB (CB (CB (CB (CB (CB (CB (C	GLU A GLU A GLU A GLU A GLU A	448 448 448		56.066 57.017 57.845 55.592 54.507	34.346 35.375 35.036 33.541 32.502	6.817 6.270 5.447 5.587 5.845	1.00 36.63 1.00 36.08 1.00 35.92 1.00 37.55 1.00 42.12
60	ATOM ATOM ATOM ATOM ATOM	3404 3405 3406 3407 3408	OE1 (OE2 (N I	GLU A GLU A GLU A LEU A LEU A	448 448 449	•	55.086 55.945 54.703 56.898 57.825	31.151 31.107 30.139 36.629 37.606	6.204 7.129 5.534 6.673 6.149	1.00 48.74 1.00 50.57 1.00 52.73 1.00 34.96
65	ATOM ATOM ATOM ATOM ATOM	3409 3410 3411 3412	C I O I CB I	EU A EU A EU A	449 449 449 449		59.294 60.147 57.429 56.115 55.677	37.265 37.251 39.023 39.457 40.857	6.502 5.621 6.552 5.858 6.339	1.00 34.44 1.00 34.44 1.00 33.97 1.00 33.23 1.00 35.54
70	ATOM ATOM ATOM	3414 3415	CD2 L	EU A SN A SN A	449 450		56.138 59.586 60.928	39.422 37.025 36.689	4.295 7.775 8.241	1.00 35.36 1.00 34.45 1.00 34.23 1.00 34.36

	ATOM	3417 3418	C O	ASN A ASN A		60.603 60.626	35.979 36.601	9.541 10.586	1.00 33.70 1.00 31.73
	ATOM ATOM	3419	CB	ASN A		61.811	37.938	8.517	1.00 35.46
	ATOM	3420	CG	ASN A		61.785	39.000	7.379	1.00 39.31
5	ATOM	3421		ASN A		62.830	39.335	6.764	1.00 42.36 1.00 39.73
	MOTA MOTA	3422 3423	ND2 N	ASN A PRO A		60.612 60.305	39.545 34.684	7.120 9.480	1.00 34.50
	ATOM	3424	CA	PRO A		59.725	33.963	10.625	1.00 35.42
	ATOM	3425	Ç	PRO A		60.614	33.694	11.792	1.00 35.46
10	ATOM	3426	O CB	PRO A		60.088 59.318	33.430 32.608	12.863 10.041	1.00 35.48 1.00 35.72
	ATOM ATOM	3427 3428	CG	PRO A		59.652	32.646	8.570	1.00 33.72
	ATOM	3429	CD	PRO A		60.536	33.793	8.322	1.00 35.07
	MOTA	3430	N	GLU A		61.918	33.728	11.606	1.00 36.10
15	ATOM ATOM	3431 3432	CA C	GLU A		62.809 63.138	33.444 34.796	12.697 13.333	1.00 37.19 1.00 35.91
	ATOM	3433	Ö	GLU A		63.356	34.883	14.500	1.00 36.70
	ATOM	3434	CB	GLU A	452	64.066	32.697	12.202	1.00 38.95
	MOTA	3435	CG	GLU A		63.927	31.164	12.122	1.00 44.32
20	ATOM ATOM	3436 3437	CD OF1	GLU A		63.457 62.294	30.631 30.923	10.758 10.354	1.00 51.15 1.00 53.26
	ATOM	3438		GLU A		64.256	29.892	10.089	1.00 56.31
	ATOM	3439	N	ARG A	453	63.120	35.878	12.579	1.00 34.02
25	MOTA	3440	CA	ARG A		63.451	37.157	13.189	1.00 32.24
25	ATOM ATOM	3441 3442	C	ARG A		62.219 62.326	37.953 38.802	13.712 14.597	1.00 31.58 1.00 30.26
	ATOM	3443	СВ	ARG A		64.186	38.017	12.182	1.00 31.61
	ATOM	3444	CG	ARG A	453	64.295	39.448	12.600	1.00 32.11
20	MOTA	3445	CD	ARG A		65.075 65.181	40.301 41.697	11.626 12.055	1.00 33.78 1.00 32.76
30	ATOM ATOM	3446 3447	NE CZ	ARG A		65.862	42.602	11.380	1.00 32.78
	ATOM	3448		ARG A		66.501	42.213	10.296	1.00 29.81
	MOTA	3449		ARG A		65.951	43.881	11.793	1.00 31.21
35	ATOM ATOM	3450 3451	N CA	CYS A		61.061 59.876	37.664 38.453	13.147 13.396	1.00 30.42 1.00 29.70
33	ATOM	3452	CA	CYS A		58.670	37.649	13.738	1.00 29.35
	ATOM	3453	Ō	CYS A	454	58.098	37.039	12.867	1.00 30.20
	ATOM	3454	CB	CYS A		59.579	39.262	12.163 11.951	1.00 29.27 1.00 29.63
40	ATOM ATOM	3455 3456	SG N	CYS A GLN A		60.790 58.269	40.536 37.693	15.005	1.00 29.03
10	ATOM	3457	CA	GLN A		57.087	36.993	15.516	1.00 29.05
	ATOM	3458	C	GLN A		56.162	37.906	16.337	1.00 28.56
	ATOM ATOM	3459 3460	O CB	GLN A		55.245 57.493	37.423 35.796	16.997 16.368	1.00 29.64 1.00 28.83
45	ATOM	3461	CG	GLN A		58.178	34.676	15.550	1.00 30.86
	ATOM	3462	CD	GLN A	455	59.028	33.712	16.408	1.00 33.92
	ATOM	3463		GLN A		58.881	33.616	17.639 15.756	1.00 36.61
	MOTA MOTA	3464 3465	NEZ N	GLN A TYR A		59.909 56.381	39.216	16.289	1.00 38.34 1.00 27.49
50	ATOM	3466	CA	TYR A		55.570	40.163	17.053	1.00 26.38
	ATOM	3467	C	TYR A		55.436	41.437	16.272	1.00 25.33
	ATOM ATOM	3468 3469	O CB	TYR A		56.342 56.265	42.254 40.497	16.278 18.391	1.00 26.26 1.00 26.47
	ATOM	3470	CG	TYR A		55.357	41.032	19.483	1.00 23.54
55	ATOM	3471		TYR A		54.969	42.361	19.514	1.00 22.01
	ATOM	3472		TYR A		54.938	40.205	20.510	1.00 22.91
	ATOM ATOM	3473 3474	CE1	TYR A		54.181 54.126	42.876 40.684	20.588 21.551	1.00 23.76 1.00 24.99
	ATOM	3475	CZ	TYR A		53.755	42.019	21.581	1.00 24.52
60	ATOM	3476	ОН	TYR A	456	52.958	42.443	22.623	1.00 32.80
	ATOM	3477	N	TYR A		54.298	41.627	15.643	1.00 24.21
	MOTA MOTA	3478 3479	CA C	TYR A		54.063 52.990	42.767 43.731	14.773 15.313	1.00 23.89 1.00 24.27
	ATOM	3480	õ	TYR A		52.067	43.282	16.028	1.00 23.48
65	MOTA	3481	CB	TYR A	457	53.524	42.197	13.454	1.00 24.73
	MOTA	3482	CG CD1	TYR A		54.585	41.559	12.548	1.00 25.26
	MOTA MOTA	3483 3484		TYR A		55.297 54.812	42.334 40.204	11.675 12.549	1.00 25.50 1.00 25.73
	ATOM	3485		TYR A		56.237	41.807	10.827	1.00 29.31
70	MOTA	3486	CE2	TYR A	457	55.769	39.642	11.701	1.00 26.68

ATOM 3492 O SER A 458 52.877 46.344 12.906 1.00 21.7 ATOM 3494 OS SER A 458 52.258 47.064 1.189 1.00 21.4 ATOM 3495 N VAL A 459 50.981 47.385 11.400 21.0 ATOM 3496 CA VAL A 459 50.981 47.385 11.400 21.0 ATOM 3497 C VAL A 459 50.981 47.385 11.400 21.0 ATOM 3498 O VAL A 459 50.197 49.285 12.149 1.00 22.9 ATOM 3498 CB VAL A 459 49.449 49.613 11.052 1.00 21.0 ATOM 3498 CG VAL A 459 49.782 47.064 11.372 1.00 21.0 ATOM 3498 CB VAL A 459 49.782 47.064 11.372 1.00 21.0 ATOM 3500 CG1 VAL A 459 48.322 47.173 11.992 1.00 21.0 ATOM 3500 CG2 VAL A 459 48.322 47.173 11.992 1.00 21.0 ATOM 3500 CA SER A 460 50.554 50.081 11.372 1.00 23.9 ATOM 3500 C SER A 460 50.554 50.081 11.372 1.00 23.9 ATOM 3500 C SER A 460 50.554 50.081 11.372 1.00 23.9 ATOM 3500 C SER A 460 50.554 50.081 11.372 1.00 22.5 ATOM 3500 C SER A 460 50.985 51.602 9.488 1.00 22.5 ATOM 3500 C SER A 460 50.985 52.509 11.301 1.00 22.5 ATOM 3500 C SER A 460 50.985 52.509 11.301 1.00 22.5 ATOM 3500 C SER A 460 50.985 52.509 11.301 1.00 22.5 ATOM 3500 C SER A 460 50.985 52.509 11.301 1.00 22.5 ATOM 3500 C SER A 460 50.985 52.509 11.301 1.00 22.5 ATOM 3500 C SER A 460 50.985 52.509 11.301 1.00 22.5 ATOM 3500 C SER A 460 50.985 52.509 11.301 1.00 25.7 ATOM 3500 C SER A 460 50.985 52.509 11.301 1.00 25.7 ATOM 3500 C SER A 460 50.985 52.509 11.301 1.00 25.7 ATOM 3500 C SER A 460 50.985 52.509 11.301 1.00 25.7 ATOM 3500 C SER A 460 50.985 52.509 11.301 1.00 25.7 ATOM 3500 C SER A 460 50.985 52.509 11.301 1.00 25.7 ATOM 3500 C SER A 460 50.985 52.509 11.301 1.00 25.7 ATOM 3500 C SER A 460 50.985 52.509 11.301 1.00 25.7 ATOM 3500 C SER A 460 50.985 52.509 11.301 1.00 25.7 ATOM 3500 C SER A 460 50.985 52.509 11.301 1.00 25.7 ATOM 3500 C SER A 460 50.985 52.509 11.301 1.00 25.7 ATOM 3500 C SER A 460 50.985 52.509 11.301 1.00 25.7 ATOM 3500 C SER A 460 50.985 52.509 11.301 1.00 25.7 ATOM 3500 C SER A 460 50.985 52.509 11.301 1.00 25.7 ATOM 3500 C SER A 460 50.985 52.509 11.00 20.7 ATOM 3500 C SER A 460 50.985 52.500 1.00 20.7 ATOM 3500 C SE	5	ATOM ATOM ATOM ATOM ATOM	3487 3488 3489 3490 3491	OH T N S CA S	YR ER ER	A 457 A 457 A 458 A 458 A 458	56.470 57.408 53.151 52.075 52.007	40.006 45.028 45.987	9.979 15.011 15.118	1.00 28.29 1.00 23.41 1.00 24.13
ATOM 3499 C A VAL A 459	·	ATOM ATOM ATOM	3492 3493 3494	O S CB S OG S	ER ER ER	A 458 A 458 A 458	52.877 52.258 53.293	46.344 47.064 47.909	12.906 16.189 15.806	1.00 23.05 1.00 21.75 1.00 23.41 1.00 26.48
ATOM 3500 CCI VAL A 459 48.332 47.173 11.992 1.00 23.9 ATOM 3501 CC2 VAL A 459 49.776 47.518 9.941 1.00 23.9 ATOM 3503 CA SER A 460 50.554 50.081 11.132 1.00 23.9 ATOM 3503 CA SER A 460 50.554 50.081 11.132 1.00 23.9 ATOM 3504 CS SER A 460 49.569 51.602 9.448 1.00 25.9 ATOM 3506 CB SER A 460 50.955 51.411 10.922 1.00 24.9 ATOM 3506 CB SER A 460 50.985 52.509 11.301 1.00 25.7 ATOM 3508 N PHE A 461 48.252 51.754 9.339 1.00 26.7 ATOM 3508 N PHE A 461 48.252 51.754 9.339 1.00 26.7 ATOM 3508 N PHE A 461 47.633 51.920 8.026 1.00 27.3 ATOM 3501 C PHE A 461 47.633 51.920 8.026 1.00 28.5 ATOM 3511 O PHE A 461 47.054 54.190 8.443 1.00 28.5 ATOM 3511 O PHE A 461 47.054 54.190 8.443 1.00 28.5 ATOM 3513 CG PHE A 461 46.299 49.777 7.822 1.00 25.2 ATOM 3513 CG PHE A 461 46.299 49.777 7.822 1.00 25.2 ATOM 3514 CDI PHE A 461 46.299 49.777 7.822 1.00 25.2 ATOM 3515 CD2 PHE A 461 46.299 49.777 7.822 1.00 25.2 ATOM 3515 CD2 PHE A 461 46.299 49.777 7.822 1.00 27.6 ATOM 3515 CD2 PHE A 461 46.299 49.777 7.822 1.00 27.6 ATOM 3515 CD2 PHE A 461 46.299 49.777 7.822 1.00 27.6 ATOM 3518 CD1 PHE A 461 46.291 49.241 6.552 1.00 27.1 ATOM 3518 CD1 PHE A 461 46.291 49.750 8.894 1.00 2.5 2.2 ATOM 3518 CD2 PHE A 461 46.291 49.750 8.894 1.00 2.5 2.2 ATOM 3518 CD2 PHE A 461 46.291 49.750 8.894 1.00 2.5 2.2 ATOM 3518 CD2 PHE A 461 46.291 49.241 6.552 1.00 27.1 ATOM 3519 CD2 PHE A 461 46.327 48.920 8.894 1.00 2.5 2.7 ATOM 3519 CD2 PHE A 461 46.291 49.241 6.552 1.00 27.1 ATOM 3519 CD2 PHE A 461 46.291 49.241 6.552 1.00 27.1 ATOM 3519 CD2 PHE A 461 46.291 49.241 6.552 1.00 27.5 ATOM 3510 CD2 PHE A 461 46.291 49.241 6.552 1.00 27.1 ATOM 3510 CD2 PHE A 461 46.291 49.241 6.552 1.00 27.5 ATOM 3510 CD2 PHE A 461 46.291 49.241 6.552 1.00 27.2 ATOM 3521 CD2 PHE A 461 46.291 49.241 6.552 1.00 27.2 ATOM 3521 CD2 PHE A 461 46.291 49.241 6.552 1.00 27.2 ATOM 3521 CD2 PHE A 461 46.291 49.241 6.552 1.00 27.2 ATOM 3521 CD2 PHE A 461 46.291 49.241 6.552 1.00 27.2 ATOM 3521 CD2 PHE A 461 46.291 49.241 6.552 1.00 27.2 ATOM 3521 CD2 PHE A 461 46.291 49.241 6.552 1.00 2	10	ATOM ATOM ATOM	3496 3497 3498	CA V C V O V	AL AL AL	A 459 A 459 A 459	50.780 50.197 49.449	47.908 49.285 49.613	12.144 12.149 13.051	1.00 22.91 1.00 23.22 1.00 20.96
ATOM 3504 C SER A 460	15	ATOM ATOM ATOM	3500 3501 3502	CG1 V CG2 V N S	AL . AL . ER .	A 459 A 459 A 460	48.322 49.776 50.554	47.173 47.518 50.081	11.992 9.941 11.132	1.00 20.67 1.00 23.93 1.00 23.90
ATOM 3509 CA PHE A 461	20	MOTA MOTA	3505 3506	C S O S CB S	ER 1 ER 1 ER 1	A 460 A 460 A 460	49.569 50.391 50.985	51.602 51.569 52.509	9.488 8.550 11.301	1.00 25.93 1.00 22.55 1.00 25.72
ATOM 3512 CB PHE A 461 46.293 51.252 8.034 1.00 25.25 ATOM 3513 CG PHE A 461 46.293 49.777 7.822 1.00 25.25 ATOM 3515 CD2 PHE A 461 46.294 49.777 7.822 1.00 27.65 ATOM 3516 CD1 PHE A 461 46.327 48.920 8.894 1.00 27.65 ATOM 3516 CE2 PHE A 461 46.327 48.920 8.894 1.00 27.65 ATOM 3517 CE2 PHE A 461 46.329 47.570 8.713 1.00 25.76 ATOM 3518 CZ PHE A 461 46.329 47.570 8.713 1.00 25.76 ATOM 3519 N SER A 462 47.631 53.691 6.347 1.00 28.77 ATOM 3519 N SER A 462 47.631 53.691 6.347 1.00 29.97 ATOM 3520 CA SER A 462 47.246 54.988 5.778 1.00 30.27 ATOM 3521 C SER A 462 47.937 55.127 5.749 1.00 30.27 ATOM 3520 CA SER A 462 47.937 55.127 5.749 1.00 30.72 ATOM 3523 CB SER A 462 47.937 55.097 4.329 1.00 30.72 ATOM 3524 OG SER A 462 46.950 54.280 3.490 1.00 38.63 ATOM 3525 N LYS A 463 43.799 56.526 5.293 1.00 35.96 ATOM 3526 CA LYS A 463 43.395 55.681 4.120 1.00 36.37 ATOM 3520 CB LYS A 463 44.018 55.519 3.05 1.00 36.37 ATOM 3520 CB LYS A 463 44.018 55.519 3.05 1.00 36.37 ATOM 3520 CB LYS A 463 44.018 55.519 3.05 1.00 36.37 ATOM 3520 CB LYS A 463 44.018 55.519 3.05 1.00 36.37 ATOM 3520 CB LYS A 463 44.018 55.519 3.05 1.00 36.37 ATOM 3520 CB LYS A 463 44.018 55.519 3.05 1.00 36.37 ATOM 3520 CB LYS A 463 44.018 55.519 3.05 1.00 36.63 ATOM 3530 CG LYS A 463 44.918 55.519 3.05 1.00 36.63 ATOM 3531 CD LYS A 463 44.918 55.519 3.05 1.00 36.63 ATOM 3533 NZ LYS A 463 44.918 55.519 3.05 1.00 35.63 ATOM 3531 CD LYS A 463 44.935 60.236 6.432 1.00 45.02 ATOM 3533 NZ LYS A 463 44.935 62.107 7.780 1.00 48.64 ATOM 3536 CB GLU A 464 42.335 52.989 3.114 1.00 33.42 ATOM 3537 CB GLU A 464 42.335 52.989 3.114 1.00 33.42 ATOM 3538 CB GLU A 464 41.549 54.257 3.209 1.00 35.63 ATOM 3536 CB GLU A 464 41.549 54.257 3.209 1.00 35.63 ATOM 3537 CB GLU A 464 42.350 52.989 3.114 1.00 33.42 ATOM 3540 CD GLU A 464 41.473 54.978 1.849 1.00 36.66 ATOM 3541 CB GLU A 464 41.178 55.783 1.625 1.00 41.82 ATOM 3543 N ALAA A 465 44.907 50.355 5.483 1.00 49.22 BATOM 3540 CD GLU A 466 47.192 51.68 1.00 31.00 31.42 ATOM 3540 CD GLU A 466 47.192 51.168 1.00 31.00 31.42 ATOM	25	ATOM ATOM	3509 3510 3511	N P CA P C P	HE A	A 461 A 461 A 461	48.252 47.633 47.418	51.754 51.920 53.377	9.329 8.026 7.628	1.00 26.78 1.00 27.31 1.00 28.08
ATOM 3516 CE1 PHE A 461 46.191 47.888 6.350, 1.00 25.376 ATOM 3518 CZ PHE A 461 46.271 47.570 8.713 1.00 25.376 ATOM 3518 N SER A 462 47.631 53.691 6.347 1.00 29.97 ATOM 3520 CA SER A 462 47.631 53.691 6.347 1.00 29.97 ATOM 3521 C SER A 462 47.246 54.988 5.778 1.00 30.27 ATOM 3522 O SER A 462 44.993 54.176 5.972 1.00 30.23 ATOM 3522 O SER A 462 44.993 54.176 5.972 1.00 30.83 ATOM 3523 CB SER A 462 44.993 54.176 5.972 1.00 30.83 ATOM 3525 N LYS A 463 45.240 56.313 5.429 1.00 33.83 ATOM 3525 N LYS A 463 45.240 56.313 5.429 1.00 33.73 ATOM 3526 CA LYS A 463 43.799 56.526 5.293 1.00 35.96 ATOM 3527 C LYS A 463 43.305 55.681 4.120 1.00 36.37 ATOM 3528 O LYS A 463 44.018 55.519 3.105 1.00 38.14 ATOM 3529 CB LYS A 463 43.492 58.014 5.103 1.00 36.63 ATOM 3530 CG LYS A 463 43.492 58.014 5.103 1.00 36.63 ATOM 3531 CD LYS A 463 44.403 58.902 5.944 1.00 39.71 ATOM 3532 CE LYS A 463 44.530 60.660 7.780 1.00 48.64 ATOM 3533 NZ LYS A 463 44.530 60.660 7.780 1.00 48.63 ATOM 3534 N GLU A 464 42.132 55.080 4.269 1.00 35.33 ATOM 3535 CA GLU A 464 42.350 52.989 3.114 1.00 33.42 ATOM 3537 O GLU A 464 42.350 52.989 3.114 1.00 33.42 ATOM 3538 CB GLU A 464 42.350 52.989 3.114 1.00 33.42 ATOM 3539 CG GLU A 464 42.350 52.989 3.114 1.00 33.42 ATOM 3539 CG GLU A 464 42.350 52.989 3.114 1.00 33.42 ATOM 3539 CG GLU A 464 42.350 52.989 3.114 1.00 33.42 ATOM 3534 N GLU A 464 42.350 52.989 3.114 1.00 33.42 ATOM 3535 CA GLU A 464 42.350 52.989 3.114 1.00 33.42 ATOM 3536 C GLU A 464 42.350 52.989 3.114 1.00 33.42 ATOM 3537 O GLU A 464 38.959 54.483 2.310 1.00 36.66 ATOM 3540 CD GLU A 464 38.959 54.483 2.310 1.00 35.66 ATOM 3541 CBI GLU A 464 38.959 54.483 2.310 1.00 32.42 ATOM 3540 CD GLU A 464 42.350 52.989 3.114 1.00 33.42 ATOM 3540 CD GLU A 464 40.178 55.783 1.625 1.00 30.626 ATOM 3540 CD GLU A 464 42.350 52.981 3.104 1.00 33.42 ATOM 3540 CD GLU A 464 42.350 52.981 3.104 1.00 33.42 ATOM 3540 CD GLU A 464 42.350 52.981 3.104 1.00 32.42 ATOM 3540 CD GLU A 465 44.765 51.681 3.093 1.00 32.42 ATOM 3554 C ALA A 465 44.765 51.681 3.093 1.00 31.60 AT	٠.	ATOM ATOM ATOM	3513 3514 3515	CG PI CD1 PI CD2 PI	HE A HE A	A 461 A 461 A 461	46.273 46.299 46.201 46.327	51.252 49.777 49.241	8.034 7.822 6.552	1.00 26.92 1.00 25.25 1.00 27.14
ATOM 3521 C SER A 462 45.723 55.127 5.749 1.00 30.27 ATOM 3522 O SER A 462 44.993 54.176 5.972 1.00 30.72 ATOM 3523 CB SER A 462 44.993 54.176 5.972 1.00 30.72 ATOM 3523 CB SER A 462 46.950 54.280 3.490 1.00 28.63 ATOM 3525 N LYS A 463 45.240 56.313 5.429 1.00 33.73 ATOM 3526 CA LYS A 463 43.799 56.526 5.293 1.00 35.76 ATOM 3527 C LYS A 463 43.305 55.681 4.120 1.00 36.37 ATOM 3529 CD LYS A 463 43.305 55.519 3.105 1.00 38.14 ATOM 3529 CG LYS A 463 43.492 58.014 5.103 1.00 36.63 ATOM 3531 CD LYS A 463 44.018 55.519 3.105 1.00 38.14 ATOM 3532 CE LYS A 463 44.03 58.902 5.944 1.00 39.71 ATOM 3533 NZ LYS A 463 44.530 60.660 7.780 1.00 48.64 ATOM 3533 NZ LYS A 463 44.530 60.660 7.780 1.00 48.64 ATOM 3533 NZ LYS A 463 44.530 60.660 7.780 1.00 48.64 ATOM 3535 CA GLU A 464 42.132 55.080 4.269 1.00 35.63 ATOM 3535 CA GLU A 464 42.132 55.080 4.269 1.00 35.63 ATOM 3537 O GLU A 464 42.132 55.080 4.269 1.00 35.63 ATOM 3538 CB GLU A 464 42.132 55.080 4.269 1.00 35.63 ATOM 3538 CB GLU A 464 42.132 55.080 4.269 1.00 35.63 ATOM 3538 CB GLU A 464 42.132 55.080 4.269 1.00 35.63 ATOM 3539 CG GLU A 464 42.132 55.080 4.269 1.00 35.63 ATOM 3534 N GLU A 464 42.132 55.080 4.269 1.00 35.63 ATOM 3535 CA GLU A 464 42.132 55.080 4.269 1.00 35.63 ATOM 3534 N GLU A 464 42.132 55.080 4.269 1.00 35.63 ATOM 3534 N GLU A 464 42.132 55.080 4.269 1.00 35.63 ATOM 3535 CA GLU A 464 42.132 55.080 4.269 1.00 35.65 ATOM 3536 C GLU A 464 42.132 55.080 4.269 1.00 35.66 ATOM 3538 CB GLU A 464 41.473 54.978 1.849 1.00 36.66 ATOM 3539 CG GLU A 464 42.107 52.137 2.259 1.00 32.17 ATOM 3534 N ALA A 465 43.279 50.500 4.737 1.00 32.17 ATOM 3540 CD GLU A 464 40.178 55.783 1.625 1.00 41.82 50.00 ATOM 3540 CD GLU A 464 40.178 55.783 1.625 1.00 41.82 50.00 ATOM 3540 CD GLU A 464 40.178 55.783 1.625 1.00 41.82 50.00 ATOM 3540 CD GLU A 464 40.00 50.56 50.00 ATOM 3540 CD GLU A 466 40.00 50.56 50.00 ATOM 3540 CD GLU A 466 40.00 50.56 50.00 50.50 4.737 1.00 32.12 ATOM 3540 CD GLU A 466 40.00 50.56 50.00 50.50 4.737 1.00 32.12 ATOM 3540 CD GLU A 466 40.00 50.56 50.00 50.50	30	ATOM ATOM ATOM	3517 3518 3519	CE2 PI CZ PI N SI	HE A HE A ER A	461 461 462	46.329 46.271	47.570 47.045	8.713 7.447	1.00 25.35 1.00 25.76 1.00 28.77
ATOM 3524 OG SER A 462 ATOM 3525 N LYS A 463 ATOM 3525 CA LYS A 463 ATOM 3526 CA LYS A 463 ATOM 3527 C LYS A 463 ATOM 3528 O LYS A 463 ATOM 3529 CB LYS A 463 ATOM 3529 CB LYS A 463 ATOM 3530 CG LYS A 463 ATOM 3531 CD LYS A 463 ATOM 3531 CD LYS A 463 ATOM 3532 CE LYS A 463 ATOM 3532 CE LYS A 463 ATOM 3533 NZ LYS A 463 ATOM 3534 N GLU A 464 ATOM 3535 CA GLU A 464 ATOM 3535 CB GLU A 464 ATOM 3537 O GLU A 464 ATOM 3538 CB GLU A 464 ATOM 3539 CG GLU A 464 ATOM 3539 CG GLU A 464 ATOM 3539 CG GLU A 464 ATOM 3536 C GLU A 464 ATOM 3537 O GLU A 464 ATOM 3538 CB GLU A 464 ATOM 3539 CG GLU A 464 ATOM 3539 CG GLU A 464 ATOM 3530 CG GLU A 464 ATOM 3530 CG GLU A 464 ATOM 3531 CD LYS A 463 ATOM 3535 CA GLU A 464 ATOM 3535 CB GLU A 464 ATOM 3536 C GLU A 464 ATOM 3537 O GLU A 464 ATOM 3538 CB GLU A 464 ATOM 3539 CG GLU A 464 ATOM 3539 CG GLU A 464 ATOM 3539 CG GLU A 464 ATOM 3540 CD GLU A 464 ATOM 3541 OE1 GLU A 464 ATOM 3540 CD GLU A 464 ATOM 3540 CD GLU A 464 ATOM 3541 OE1 GLU A 464 ATOM 3540 CD GLU A 464 ATOM 3541 OE1 GLU A 464 ATOM 3540 CD GLU A 464 ATOM 3541 OE1 GLU A 464 ATOM 3540 CD GLU A 464 ATOM 3541 OE1 GLU A 464 ATOM 3542 OE2 GLU A 464 ATOM 3543 N ALA A 465 ATOM 3544 CA ALA A 465 ATOM 3545 C ALA A 465 ATOM 3545 C ALA A 465 ATOM 3546 O ALA A 465 ATOM 3547 CB ALA A 465 ATOM 3548 N LYS A 466 ATOM 3548 N LYS A 466 ATOM 3548 N LYS A 466 ATOM 3549 CA LYS A 466 ATOM 3540 CD LYS A 466 ATOM 3540 CD LYS A 466 ATOM 35540 C LYS A 466 ATOM 3554	35	ATOM ATOM	3521 3522	C SI	ER A	462 462	45.723 44.993	55.127 54.176	5.749 5.972	1.00 30.27 1.00 31.48 1.00 30.72
ATOM 3529 CB LYS A 463	40	ATOM ATOM ATOM	3525 3526 3527	CA LY	S A	463 463 463	45.240 43.799 43.305	56.313 56.526 55.681	3.490 5.429 5.293 4.120	1.00 28.63 1.00 33.73 1.00 35.96 1.00 36.37
ATOM 3534 N GLU A 464 42.132 55.080 4.269 1.00 35.63 ATOM 3535 CA GLU A 464 41.549 54.257 3.209 1.00 35.32 50 ATOM 3536 C GLU A 464 42.350 52.989 3.114 1.00 33.42 ATOM 3537 O GLU A 464 42.107 52.137 2.259 1.00 32.17 ATOM 3538 CB GLU A 464 41.473 54.978 1.849 1.00 36.66 ATOM 3539 CG GLU A 464 40.178 55.783 1.625 1.00 41.82 ATOM 3540 CD GLU A 464 38.919 54.943 1.348 1.00 49.22 55 ATOM 3541 OE1 GLU A 464 38.556 54.770 0.164 1.00 50.56 ATOM 3542 OE2 GLU A 464 38.556 54.770 0.164 1.00 50.56 ATOM 3543 N ALA A 465 43.302 52.871 4.031 1.00 32.42 ATOM 3544 CA ALA A 465 44.115 51.683 4.130 1.00 31.60 ATOM 3546 C ALA A 465 44.115 51.683 4.130 1.00 31.60 ATOM 3546 O ALA A 465 44.746 51.223 2.805 1.00 30.62 60 ATOM 3546 O ALA A 465 44.746 51.223 2.805 1.00 30.62 ATOM 3548 N LYS A 466 47.46 51.223 2.805 1.00 32.12 ATOM 3549 CA LYS A 466 45.108 52.139 1.934 1.00 31.42 ATOM 3550 C LYS A 466 45.748 51.643 0.743 1.00 32.12 ATOM 3551 O LYS A 466 47.687 50.345 0.299 1.00 30.10 ATOM 3552 CB LYS A 466 47.687 50.345 0.299 1.00 30.10 ATOM 3552 CB LYS A 466 45.656 52.630 -0.428 1.00 33.58	45	ATOM ATOM ATOM ATOM	3529 3530 3531 3532	CB LY CD LY CE LY	S A S A S A	463 463 463 463	43.492 44.403 43.822 44.530	58.014 58.902 60.236 60.660	5.103 5.944 6.432	
ATOM 3538 CB GLU A 464 41.473 54.978 1.849 1.00 36.66 ATOM 3539 CG GLU A 464 40.178 55.783 1.625 1.00 41.82 ATOM 3540 CD GLU A 464 38.919 54.943 1.348 1.00 49.22 55 ATOM 3541 OE1 GLU A 464 38.556 54.770 0.164 1.00 50.56 ATOM 3542 OE2 GLU A 464 38.259 54.483 2.310 1.00 53.57 ATOM 3543 N ALA A 465 43.302 52.871 4.031 1.00 32.42 ATOM 3544 CA ALA A 465 44.115 51.683 4.130 1.00 31.60 ATOM 3545 C ALA A 465 44.746 51.223 2.805 1.00 30.62 60 ATOM 3546 O ALA A 465 44.907 50.035 2.563 1.00 27.72 ATOM 3548 N LYS A 466 45.748 51.643 0.743 1.00 32.19 ATOM 3549 CA LYS A 466 45.748 51.643 0.743 1.00 32.19 ATOM 3550 C LYS A 466 47.192 51.168 1.038 1.00 31.32 65 ATOM 3551 O LYS A 466 47.687 50.345 0.299 1.00 30.10 ATOM 3552 CB LYS A 466 47.687 50.345 0.299 1.00 30.10 ATOM 3552 CB LYS A 466 45.656 52.630 -0.428 1.00 33.58	50	ATOM ATOM ATOM	3534 3535 3536	N GL CA GL C GL	U A U A U A	464 464 464	42.132 41.549 42.350	55.080 54.257 52.989	4.269 3.209 3.114	1.00 35.32 1.00 33.42
ATOM 3544 CA ALA A 465 44.115 51.683 4.130 1.00 31.60 ATOM 3545 C ALA A 465 44.746 51.223 2.805 1.00 30.62 ATOM 3546 O ALA A 465 44.907 50.035 2.563 1.00 27.72 ATOM 3547 CB ALA A 465 43.279 50.550 4.737 1.00 32.19 ATOM 3548 N LYS A 466 45.108 52.139 1.934 1.00 31.42 ATOM 3549 CA LYS A 466 45.748 51.643 0.743 1.00 32.12 ATOM 3550 C LYS A 466 47.192 51.168 1.038 1.00 31.32 ATOM 3551 O LYS A 466 47.687 50.345 0.299 1.00 30.10 ATOM 3552 CB LYS A 466 45.656 52.630 -0.428 1.00 33.58	55	ATOM ATOM ATOM ATOM ATOM	3538 3539 3540 3541 3542	CB GL CG GL CD GL OE1 GL OE2 GL	U A U A U A U A U A	464 464 464 464	41.473 40.178 38.919 38.556 38.259	54.978 55.783 54.943 54.770 54.483	1.849 1.625 1.348 0.164 2.310	1.00 36.66 1.00 41.82 1.00 49.22 1.00 50.56 1.00 53.57
ATOM 3548 N LYS A 466 45.108 52.139 1.934 1.00 31.42 ATOM 3549 CA LYS A 466 45.748 51.643 0.743 1.00 32.12 ATOM 3550 C LYS A 466 47.192 51.168 1.038 1.00 31.32 65 ATOM 3551 O LYS A 466 47.687 50.345 0.299 1.00 30.10 ATOM 3552 CB LYS A 466 45.656 52.630 -0.428 1.00 33.58	60	ATOM ATOM ATOM	3544 3545 3546	CA AL C AL O AL	A A A A A A	465 465 465	44.115 44.746 44.907	51.683 51.223 50.035	4.130 2.805 2.563	1.00 31.60 1.00 30.62 1.00 27.72
AMON 3553 GG THG 3 466	65	ATOM ATOM ATOM ATOM	3548 3549 3550 3551	N LY CA LY C LY O LY	S A S A S A	466 466 466 466	45.108 45.748 47.192 47.687	52.139 51.643 51.168 50.345	1.934 0.743 1.038 0.299	1.00 31.42 1.00 32.12 1.00 31.32
ATOM 3554 CD LYS A 466 43.427 51.805 -1.556 1.00 43.92 ATOM 3555 CE LYS A 466 41.904 52.062 -1.554 1.00 47.17 70 ATOM 3556 NZ LYS A 466 41.126 51.288 -2.589 1.00 48.39	70	ATOM ATOM ATOM	3553 3554 3555	CG LY CD LY CE LY	S A S A S A	466 466 466	44.196 43.427 41.904	52.978 51.805 52.062	-0.869 -1.556 -1.554	1.00 38.27 1.00 43.92 1.00 47.17

	ATOM	3557	N	TYR	Α	467	47.827	51.635	2.127	1.00 31.47
	ATOM	3558	CA			467	49.198	51.263	2.498	1.00 30.89
	ATOM	3559	C			467	49.333	50.950	4.001	1.00 30.71
	ATOM	3560	Õ			467	48.572	51.497	4.829	1.00 30.78
5	ATOM	3561	CB	TYR	Α	467	50.099	52.423	2.122	1.00 31.64
	ATOM	3562	CG	TYR	Α	467	50.056	52.721	0.646	1.00 31.24
	ATOM	3563	CD1				50.704	51.896	-0.260	1.00 32.67
	ATOM	3564	CD2				49.383	53.822	0.159	1.00 30.99
	ATOM	3565	CE1			467	50.672	52.162	-1.614	1.00 34.60
10	ATOM	3566	CE2				49.333	54.093	-1.184	1.00 31.48
	ATOM	3567	CZ			467	49.976	53.257	-2.072	1.00 34.16
	ATOM	3568	OH	TYR			49.927	53.534	-3.412	1.00 34.89
	ATOM ATOM	3569 3570	N	TYR		468	50.252 50.549	50.044 49.763	4.343 5.731	1.00 29.12 1.00 28.87
15	ATOM	3570	CA C	TYR			52.062	49.763	6.052	1.00 28.87 1.00 28.68
15	ATOM	3572	Ö	TYR			52.877	49.243	5.210	1.00 28.35
	ATOM	3573	СВ			468	49.772	48.537	6.288	1.00 29.07
	ATOM	3574	CG			468	49.899	47.194	5.553	1.00 28.06
	ATOM	3575	CD1				49.122	46.912	4.438	1.00 28.62
20	MOTA	3576	CD2	TYR	Α	468	50.698	46.193	6.045	1.00 26.47
	MOTA	3577	CE1	TYR	Α	468	49.194	45.691	3.813	1.00 28.32
	ATOM	3578	CE2	TYR			50.782	44.984	5.446	1.00 26.79
	MOTA	3579	CZ	TYR			50.033	44.737	4.311	1.00 28.16
	ATOM	3580	OH	TYR			50.124	43.527	3.688	1.00 29.41
25	ATOM	3581	N	GLN			52.412	50.086	7.255	1.00 27.13
	ATOM	3582	CA	GLN			53.763	49.962	7.777	1.00 27.19
	ATOM ATOM	3583 3584	C O	GLN GLN			53.697 52.864	48.856 48.893	8.804 9.715	1.00 27.67 1.00 26.15
	ATOM	3585	СВ	GLN			54.221	51.271	8.435	1.00 20.15
30	ATOM	3586	CG	GLN			55.515	51.121	9.271	1.00 27.66
	ATOM	3587	CD	GLN			55.813	52.307	10.219	1.00 29.76
	ATOM	3588		GLN			54.907	52.829	10.922	1.00 28.34
	ATOM	3589	NE2	GLN	Α	469	57.074	52.746	10.216	1.00 23.42
	ATOM	3590	N	LEU	Α	470	54.496	47.825	8.619	1.00 28.25
35	MOTA	3591	CA	LEU			54.587	46.804	9.611	1.00 29.45
	ATOM	3592	C	LEU			55.797	47.118	10.459	1.00 30.58
	ATOM	3593	0	LEU			56.836	47.556	9.967	1.00 30.74
	ATOM	3594	CB	LEU			54.777	45.416	8.997	1.00 29.96
40	ATOM ATOM	3595 3596	CG CD1	LEU LEU			53.477 53.812	44.700 43.418	8.545 7.817	1.00 31.71 1.00 32.62
40	ATOM	3597		LEU			52.576	44.404	9.710	1.00 32.02
	ATOM	3598	N	ARG			55.667	46.868	11.740	1.00 32.00
	MOTA	3599	CA	ARG			56.770	47.057	12.635	1.00 33.21
	ATOM	3600	C	ARG			56.856	45.811	13.476	1.00 32.36
45	ATOM	3601	0	ARG	Α	471	55.922	45.448	14.189	1.00 31.00
	MOTA	3602	CB	ARG			56.614	48.363	13.390	1.00 34.66
	MOTA	3603	CG	ARG			55.836	48.362	14.607	1.00 40.62
	ATOM	3604	CD	ARG			56.698	48.373	15.909	1.00 48.15
E 0	ATOM	3605	NE	ARG			55.770	48.361	17.041	1.00 53.40
50	ATOM	3606	CZ	ARG			55.725	49.259 50.241	18.013 18.094	1.00 58.18
	ATOM ATOM	3607 3608		ARG ARG			56.628 54.785	49.148	18.937	1.00 61.35 1.00 58.39
	ATOM	3609	N	CYS			57.929	45.069	13.232	1.00 38.39
	ATOM	3610	CA	CYS			58.189	43.834	13.942	1.00 31.86
55	ATOM	3611	C	CYS			59.049	44.198	15.119	1.00 31.18
	ATOM	3612	ō	CYS			59.922	45.056	14.990	1.00 29.72
	ATOM	3613	СВ	CYS	Α	472	58.876	42.844	12.993	1.00 32.72
	ATOM	3614	SG	CYS	Α	472	60.216	41.804	13.588	1.00 34.36
	ATOM	3615	N	SER			58.755	43.566	16.248	1.00 30.57
60	MOTA	3616	CA	SER			59.372	43.858	17.532	1.00 31.00
	ATOM	3617	C	SER			60.270	42.760	18.076	1.00 30.76
	ATOM	3618	0	SER			60.819	42.915	19.159	1.00 32.46
	MOTA	3619	CB	SER			58.260	44.077	18.588	1.00 31.69
6 E	ATOM	3620	OG	SER			57.860	45.417	18.636	1.00 32.84
65	ATOM ATOM	3621 3622	N CA	GLY GLY			60.402 61.186	41.644	17.385	1.00 30.01
	ATOM	3623	CA	GLY			60.725	40.535 39.199	17.887 17.347	1.00 29.79 1.00 29.71
	ATOM	3624	0	GLY			59.682	39.139	16.739	1.00 29.71
	ATOM	3625	N	PRO			61.418	38.118	17.679	1.00 29.74
70	ATOM	3626	CA	PRO			62.509	38.114	18.663	1.00 30.22

	ATOM ATOM ATOM ATOM	3628 3629	O CB	PRO PRO	A 475 A 475 A 475 A 475		63.829 64.712 62.674 61.922	38.778 36.609	18.969 19.015	1.00 31.04 1.00 29.67
5		3631 3632 3633 3634	CD N CA	PRO GLY GLY	A 475 A 476 A 476 A 476		61.206 63.963 65.211	36.800 38.978 39.512	17.911 17.066 16.855 16.314	1.00 30.13 1.00 29.71 1.00 29.41
10	ATOM	3635 3636 3637 3638	O N	GLY LEU LEU	A 476 A 477 A 477 A 477		65.119 64.185 66.067 66.074	41.506 41.727 43.170	16.463 17.120 15.882 15.928	1.00 30.30 1.00 29.02 1.00 28.65
15	ATOM ATOM	3639 3640 3641 3642	O CB CG	LEU LEU	A 477 A 477 A 477		64.868 64.433 67.372 68.606 69.808	43.304 43.679 43.457	15.190 14.157 15.293 16.177	1.00 26.15 1.00 28.42 1.00 29.87
20	ATOM ATOM ATOM ATOM	3643 3644 3645 3646	CD2 N CA C	PRO PRO	A 477 A 478 A 478 A 478		68.505 64.337 63.171 63.419	43.864 44.276 44.870 45.506 45.825	15.412 17.417 15.724 15.103	1.00 32.61 1.00 28.72 1.00 28.98
	ATOM ATOM ATOM ATOM	3647 3648 3649 3650	O CB CG CD	PRO I	A 478 A 478 A 478		64.550 62.978 63.414 64.714	46.155 46.761 46.249 45.532	13.638 13.244 15.941 17.350	1.00 28.98 1.00 27.85 1.00 28.60 1.00 29.75
25	ATOM ATOM ATOM ATOM	3651 3652 3653 3654	N CA C	LEU A	A 479 A 479 A 479	•	62.338 62.375 61.045 59.962	45.722 45.825 46.453 45.958	16.984 12.864 11.412 10.988 11.325	1.00 29.65 1.00 28.30 1.00 27.04 1.00 26.54
30	ATOM ATOM ATOM ATOM	3655 3656 3657 3658	CB CG CD1	LEU A LEU A LEU A	479 479 479		62.564 62.972 61.838 63.598	44.428 44.059 43.399 45.165	11.323 10.862 9.438 8.745 8.607	1.00 23.86 1.00 27.50 1.00 28.18 1.00 29.02
35	ATOM ATOM ATOM ATOM	3659 3660 3661 3662	N CA C O	TYR A TYR A TYR A	480 480 480		61.172 60.084 60.084 61.123	47.592 48.394 48.347 48.628	10.317 9.838 8.311 7.682	1.00 29.05 1.00 25.53 1.00 25.57 1.00 25.69
40	ATOM ATOM ATOM ATOM	3663 3664 3665 3666	CB CG CD1	TYR A TYR A TYR A TYR A	480 480 480		60.307 60.366 61.473 59.288	49.839 49.940 49.507 50.441	10.334 11.886 12.582 12.624	1.00 24.97 1.00 26.20 1.00 26.83 1.00 26.40
	ATOM ATOM ATOM ATOM	3667 3668 3669 3670	CE1	TYR A TYR A TYR A TYR A	480 480 480		61.541 59.342 60.474 60.589	49.597 50.563 50.126	13.959 14.009 14.671	1.00 28.75 1.00 27.86 1.00 27.36 1.00 28.64
45	ATOM ATOM ATOM ATOM	3671 3672 3673 3674	N CA C	THR A THR A THR A THR A	481 481 481		58.947 58.733 57.444	50.175 47.948 47.783 48.464	16.028 7.740 6.280 5.823	1.00 32.30 1.00 25.79 1.00 25.94 1.00 26.79
50	ATOM ATOM ATOM ATOM	3675 3676 3677 3678	CB OG1 CG2	THR A THR A THR A LEU A	481 481 481		56.468 58.642 57.689 59.953	48.610 46.300 45.652 45.559	6.603 5.940 6.796 6.259	1.00 27.75 1.00 25.77 1.00 24.73 1.00 25.11
55	ATOM ATOM ATOM ATOM	3679 3680 3681 3682	CA C O CB	LEU A LEU A LEU A	482 482 482 482		57.407 56.198 55.617 56.364 56.583	48.893 49.551 48.647 47.964 50.886	4.577 4.017 2.970 2.261 3.393	1.00 27.02 1.00 28.39 1.00 29.00 1.00 28.88 1.00 28.80
60	ATOM ATOM ATOM ATOM ATOM	3684 3685 3686 3687	CD1 CD2 N	LEU A LEU A HIS A	482 482 483		55.694 55.322 54.559 54.286	52.065 52.000 52.139 48.625	3.061 1.602 4.010 2.888	1.00 29.45 1.00 34.74 1.00 31.91 1.00 29.13
65	ATOM ATOM ATOM ATOM	3688 3689 3690 3691	C I O I CB I	HIS A HIS A HIS A	483 483 483		53.561 52.327 51.631 53.058	47.745 48.347 49.183 46.565	1.987 1.339 1.928 2.774	1.00 29.27 1.00 29.70 1.00 29.62 1.00 29.56
	ATOM ATOM ATOM ATOM	3692 3693 3694	ND1 F CD2 F CE1 F	HIS A HIS A HIS A	483 483 483		54.109 54.478 54.809 55.394	45.781 46.048 44.682 45.179	3.488 4.791 3.121 5.172	1.00 30.37 1.00 32.06 1.00 29.51 1.00 28.87
70	ATOM			HIS A SER A			55.614 52.017	44.340 47.866	4.181 0.140	1.00 29.23 1.00 30.49

	ATOM	3697	CA	SER			50.780	48.273	-0.530	1.00 31.66
	ATOM	3698	С	SER	Α	484	49.644	47.255	-0.340	1.00 31.04
	ATOM	3699	Ö	SER			49.830	46.068	-0.516	1.00 29.45
		3700		SER			51.018	48.473	-2.004	1.00 31.81
_	ATOM		CB							
5	MOTA	3701	OG	SER			51.194	47.221	-2.593	1.00 36.07
	ATOM	3702	N	SER	Α	485	48.471	47.713	0.052	1.00 31.59
	ATOM	3703	CA	SER	Α	485	47.377	46.779	0.341	1.00 31.97
	ATOM	3704	C	SER			46.812	45.981	-0.889	1.00 33.22
							46.347	44.871	-0.733	1.00 31.17
	ATOM	3705	0	SER						
10	ATOM	3706	CB	SER	A	485	46.224	47.517	1.056	1.00 31.84
	ATOM	3707	OG	SER	Α	485	46.495	47.820	2.429	1.00 30.78
	ATOM	3708	N	VAL	Α	486	46.906	46.520	-2.092	1.00 35.73
	ATOM	3709	CA	VAL			46.320	45.843	-3.290	1.00 38.83
									-3.445	
	ATOM	3710	С	VAL			46.643	44.361		1.00 39.66
15	ATOM	3711	0	VAL	Α	486	45.762	43.547	-3.497	1.00 39.83
	ATOM	3712	CB	VAL	Α	486	46.779	46.461	-4.616	1.00 39.39
	ATOM	3713	CG1	VAL	А	486	45.994	45.827	-5.743	1.00 40.77
	ATOM	3714		VAL			46.560	47.936	-4.622	1.00 40.89
	ATOM	3715	N	ASN			47.918	44.043	-3.544	1.00 41.49
20	ATOM	3716	CA	ASN	A	487	48.397	42.673	-3.672	1.00 43.70
	ATOM	3717	С	ASN	Α	487	49.507	42.699	-2.646	1.00 44.54
	ATOM	3718	Ō	ASN			50.661	43.041	-2.976	1.00 47.53
	ATOM	3719	ČВ	ASN			48.968	42.424	-5.079	1.00 43.60
	-									
	ATOM	3720	CG	ASN			47.931	42.677	-6.209	1.00 46.15
25	ATOM	3721	OD1	ASN	Α	487	47.879	43.771	-6.808	1.00 45.78
	ATOM	3722	ND2	ASN	Α	487	47.090	41.666	-6.480	1.00 47.33
	ATOM	3723	N	ASP	Α	488	49.156	42.406	-1.407	1.00 44.16
		3724		ASP			49.991	42.765	-0.256	1.00 43.13
	MOTA		CA							
	MOTA	3725	С	ASP			51.440	42.640	-0.572	1.00 42.07
30	MOTA	3726	0	ASP	Α	488	52.063	41.698	-0.129	1.00 41.39
	ATOM	3727	CB	ASP	Α	488	49.632	41.919	0.969	1.00 43.40
	ATOM	3728	CG	ASP			48.261	42.269	1.535	1.00 44.42
		3729		ASP			47.250	41.758	1.016	1.00 44.23
	ATOM									
	MOTA	3730		ASP			48.113	43.048	2.498	1.00 47.17
35	MOTA	3731	N	LYS	А	489	51.970	43.591	-1.336	1.00 41.40
	MOTA	3732	CA	LYS	Α	489	53.362	43.532	-1.778	1.00 41.77
	ATOM	3733	С	LYS			54.208	44.372	-0.850	1.00 39.87
		3734		LYS			53.766	45.428	-0.402	1.00 39.61
	ATOM		0_							
	MOTA	3735	СВ	LYS			53.509	44.059	-3.223	1.00 43.04
40	ATOM	3736	CG	LYS	А	489	54.927	43.896	-3.868	1.00 45.55
	ATOM	3737	CD	LYS	Α	489	54.887	44.193	-5.389	1.00 48.94
	ATOM	3738	CE	LYS	A	489	56.304	44.463	-6.036	1.00 51.28
	ATOM	3739	NZ	LYS			56.810	45.920	-6.081	1.00 49.79
										1.00 37.79
	MOTA	3740	N	GLY			55.396	43.882	-0.532	
45	ATOM	3741	CA	GLY			56.324	44.656	0.259	1.00 37.25
	ATOM	3742	С	GLY	Α	490	56.914	45.694	-0.665	1.00 36.45
	ATOM	3743	0	GLY	А	490	57.299	45.383	-1.788	1.00 37.78
		3744		LEU						1.00 35.33
	MOTA									
	ATOM	3745	CA	LEU			57.461	47.964	-1.104	1.00 34.44
50	ATOM	3746	С	LEU	Α	491	58.935	48.323	-0.856	1.00 34.34
	ATOM	3747	0	LEU	Α	491	59.670	48.514	-1.839	1.00 34.89
	MOTA	3748	CB	LEU	А	491	56.580	49.197	-0.989	1.00 34.55
	ATOM	3749	CG	LEU			55.123	49.022	-1.451	1.00 34.62
	ATOM	3750		LEU			54.288	50.122	-0.858	1.00 33.61
55	MOTA	3751	CD2	LEU	Α	491	54.968	48.996	-2.978	1.00 31.54
	ATOM	3752	N	ARG	Α	492	59.343	48.434	0.426	1.00 32.66
	ATOM	3753	CA	ARG			60.660	48.927	0.871	1.00 31.58
		3754		ARG			60.864	48.546	2.277	1.00 30.93
	ATOM		C							
	ATOM	3755	0_	ARG			59.901	48.480	3.019	1.00 30.06
60	ATOM	3756	CB	ARG	Α	492	60.645	50.434	1.042	1.00 32.97
	ATOM	3757	CG	ARG	Α	492	60.828	51.171	-0.161	1.00 34.92
	ATOM	3758	CD	ARG			60.326	52.610	-0.150	1.00 34.50
				ARG			59.490	52.636	-1.321	1.00 32.59
	ATOM	3759	NE	ANG	Ÿ	400				
	MOTA	3760	CZ	ARG			58.219	52.906	-1.332	1.00 34.65
65	MOTA	3761		ARG			57.575	53.305	-0.232	1.00 32.87
	MOTA	3762	NH2	ARG	Α	492	57.586	52.809	-2.491	1.00 37.06
	ATOM	3763	N	VAL			62.127	48.449	2.653	1.00 30.19
		3764	CA	VAL			62.542	48.283	4.028	1.00 30.35
	ATOM									
	MOTA	3765	C	VAL			62.731	49.718	4.529	1.00 29.81
70	MOTA	3766	0	VAL	Α	493	63.407	50.499	3.881	1.00 29.10

5	MOTA MOTA MOTA MOTA	3767 3768 3769 3770 3771	CG1 VAI CG2 VAI N LEU CA LEU	A 493 JA 494 JA 494	63.861 64.339 63.706 62.112 62.266	47.465 46.116 50.085 51.451	4.125 5.601 3.602 5.653 6.148	1.00 30.28 1.00 32.53 1.00 30.23 1.00 29.29 1.00 27.76
10	ATOM ATOM ATOM ATOM ATOM	3772 3773 3774 3775 3776	O LEU	J A 494 J A 494 J A 494 J A 494	63.412 64.179 60.947 59.767 58.460	52.547 51.946 51.913	7.157 7.086 6.728 5.744 6.574	1.00 27.82 1.00 26.89 1.00 28.18 1.00 25.32 1.00 25.03
15	ATOM ATOM ATOM ATOM	3777 3778 3779 3780	CD2 LEU N GLU CA GLU C GLU	I A 494 I A 495 I A 495 I A 495	59.837 63.507 64.583 64.800	53.020 50.668 50.634 49.191	4.700 8.097 9.053 9.423	1.00 25.03 1.00 25.99 1.00 26.93 1.00 26.86 1.00 27.38
13	ATOM ATOM ATOM ATOM ATOM	3781 3782 3783 3784 3785	CB GLU	A 495 A 495 A 495 A 495 A 495	63.850 64.227 65.284 66.667 66.849	48.505 51.421 51.279 51.737 52.939	9.886 10.320 11.406 10.964 10.662	1.00 27.45 1.00 26.93 1.00 27.46 1.00 28.72 1.00 27.14
20	ATOM ATOM ATOM ATOM ATOM	3786 3787 3788 3789 3790	OE2 GLU N ASP CA ASP C ASP	A 495 A 496 A 496 A 496 A 496	67.565 66.021 66.343 67.312 67.664	50.872 48.710 47.347 47.209	10.896 9.216 9.595 10.761	1.00 32.40 1.00 26.60 1.00 27.19 1.00 26.76
25	ATOM ATOM ATOM ATOM	3791 3792 3793 3794	CB ASP CG ASP OD1 ASP OD2 ASP	A 496 A 496 A 496 A 496	66.845 68.163 68.807 68.622	46.094 46.509 46.991 47.907 46.504	11.095 8.409 7.848 8.429 6.788	1.00 25.91 1.00 27.04 1.00 30.52 1.00 35.11 1.00 32.05
30	ATOM ATOM ATOM ATOM	3795 3796 3797 3798 3799	CA ASN C ASN O ASN	A 497 A 497 A 497 A 497 A 497	67.705 68.661 69.958 70.514 67.977	48.316 48.285 47.515 46.820 47.719	11.377 12.494 12.182 13.063 13.784	1.00 27.15 1.00 28.78 1.00 29.53 1.00 29.16 1.00 29.45
35	ATOM ATOM ATOM ATOM ATOM	3800 3801 3802 3803 3804	OD1 ASN ND2 ASN N SER		67.124 67.646 65.789 70.432	48.763 49.769 48.545 47.622	14.482 14.931 14.541 10.936	1.00 30.00 1.00 29.24 1.00 29.26 1.00 29.99
40	ATOM ATOM ATOM ATOM	3805 3806 3807 3808	C SER O SER CB SER OG SER	A 498 A 498 A 498 A 498	71.712 72.841 73.730 72.055 72.035	47.020 47.552 46.819 47.346 48.768	10.552 11.438 11.855 9.088 8.935	1.00 31.47 1.00 31.80 1.00 32.35 1.00 31.18 1.00 33.29
45	ATOM ATOM ATOM ATOM ATOM	3809 3810 3811 3812 3813	CA ALA C ALA O ALA	A 499 A 499 A 499 A 499 A 499	72.798 73.828 73.919 74.989 73.590	48.834 49.425 48.707 48.185	11.730 12.546 13.900 14.270	1.00 32.02 1.00 31.95 1.00 33.04 1.00 33.43
50	ATOM ATOM ATOM ATOM ATOM	3814 3815 3816 3817 3818	N LEU CA LEU C LEU O LEU	A 500 A 500 A 500 A 500 A 500	72.794 72.779 73.212 73.939 71.365	50.888 48.580 47.942 46.496 45.975 48.041	12.681 14.605 15.907 15.818 16.662 16.494	1.00 31.12 1.00 33.98 1.00 34.37 1.00 34.56 1.00 35.16
55	ATOM ATOM ATOM ATOM ATOM	3819 3820 3821 3822 3823	CG LEU CD1 LEU CD2 LEU N ASP	A 500 A 500	71.074 70.484 72.261 72.719 73.139	47.771 46.432 47.905 45.816 44.443	17.973 18.084 18.963 14.819 14.585	1.00 36.71 1.00 38.33 1.00 36.14 1.00 35.24 1.00 36.88
60	ATOM ATOM ATOM ATOM ATOM	3824 3825 3826 3827 3828	C ASP O ASP CB ASP	A 501 A 501 A 501 A 501	74.696 75.249 72.671 72.683 71.921	44.349 43.495 43.974 42.495 41.847	14.649 15.355 13.210 13.088	1.00 36.67 1.00 35.36 1.00 37.03 1.00 41.29
65	ATOM ATOM ATOM ATOM	3829 3830 3831 3832	OD2 ASP N LYS CA LYS C LYS	A 501 A 502 A 502 A 502	73.420 75.404 76.877 77.493	41.864 45.224 45.081 45.344	13.829 12.295 13.936 13.949 15.326	1.00 47.04 1.00 48.28 1.00 36.25 1.00 36.92 1.00 35.12
70	ATOM ATOM ATOM ATOM	3833 3834 3835 3836	CB LYS	A 502 A 502 A 502 A 502	78.362 77.591 77.079 78.126	44.624 45.872 47.247 48.152	15.719 12.839 12.631 11.978	1.00 34.06 1.00 37.57 1.00 40.85 1.00 45.63

	ATOM	3837	CE	LYS	Α	502	78.246	49.438	12.847	1.00 46.85
	ATOM	3838	NZ	LYS	Α	502	76.961	49.683	13.597	1.00 42.88
	ATOM	3839	N	MET			76.995		16.087	1.00 34.82
		3840				503	77.579		17.380	1.00 35.39
_	ATOM		CA							
5	ATOM	3841	С	MET			77.372		18.285	1.00 35.75
	ATOM	3842	0	MET	Α	503	78.279	44.940	19.019	1.00 35.08
	ATOM	3843	CB	MET	Α	503	77.014	47.788	18.017	1.00 35.70
	ATOM	3844	CG	MET	Δ	503	77.302	49.022	17.252	1.00 37.65
	ATOM	3845	SD	MET			76.521	50.415	18.018	1.00 43.87
••										
10	ATOM	3846	CE	MET			74.863	50.228	17.447	1.00 44.49
	ATOM	3847	N	LEU	Α	504	76.187		18.181	1.00 36.04
	ATOM	3848	CA	LEU	Α	504	75.781	43.655	19.060	1.00 35.94
	ATOM	3849	С	LEU	Α	504	76.558	42.406	18.780	1.00 36.06
	ATOM	3850	ō	LEU			76.739		19.664	1.00 35.69
15	ATOM	3851	ČВ	LEU			74.274		18.967	1.00 36.22
13			_							
	ATOM	3852	CG	LEU			73.461	44.615	19.567	1.00 37.88
	ATOM	3853	CD1	LEU	Α	504	71.989	44.234	19.691	1.00 40.39
	ATOM	3854	CD2	LEU	Α	504	73.950	45.071	20.940	1.00 37.32
	ATOM	3855	N	GLN	Α	505	77.069	42.308	17.557	1.00 36.55
20	ATOM	3856	CA	GLN			77.963	41.218	17.220	1.00 36.93
20							79.177	41.269	18.157	1.00 35.99
	MOTA	3857	C	GLN						
	ATOM	3858	0	GLN			79.738	40.237	18.463	1.00 34.66
	ATOM	3859	CB	GLN	A	505	78.40 7	41.308	15.752	1.00 37.71
	ATOM	3860	CG	GLN	Α	505	77.323	40.933	14.739	1.00 41.41
25	ATOM	3861	CD	GLN			77.637	41.489	13.330	1.00 47.47
	ATOM	3862		GLN			78.811	41.591	12.958	1.00 52.31
		3863		GLN			76.596	41.866	12.566	1.00 48.31
	ATOM									
	ATOM	3864	N	ASN			79.584	42.457	18.605	1.00 36.22
	ATOM	3865	CA	ASN	Α	506	80.733	42.539	19.507	1.00 37.72
30	ATOM	3866	С	ASN	Α	506	80.348	42.595	20.978	1.00 37.33
	ATOM	3867	0	ASN	Α	506	81.134	43.044	21.804	1.00 36.99
	ATOM	3868	ČВ	ASN			81.685	43.699	19.196	1.00 38.48
							83.156	43.382	19.579	1.00 30.40
	ATOM	3869	CG	ASN						
	ATOM	3870		ASN			83.488	42.260	20.002	1.00 46.82
35	ATOM	3871	ND2	ASN	A	506	84.038	44.348	19.386	1.00 44.80
	ATOM	3872	N	VAL	Α	507	79.158	42.105	21.309	1.00 37.21
	ATOM	3873	CA	VAL	Α	507	78.777	42.019	22.697	1.00 36.18
	ATOM	3874	C	VAL			78.353	40.601	23.064	1.00 35.75
	MOTA	3875	0	VAL			77.729	39.885	22.272	1.00 33.24
40	ATOM	3876	CB	VAL			77.672	43.043	23.009	1.00 36.32
	ATOM	3877	CG1	VAL	Α	507	77.465	43.154	24.527	1.00 36.71
	ATOM	3878	CG2	VAL	Α	507	78.055	44.354	22.479	1.00 33.94
	ATOM	3879	N	GLN			78.723	40.155	24.262	1.00 35.82
	ATOM	3880	CA	GLN			78.250	38.829	24.703	1.00 36.41
45	ATOM	3881	C	GLN			76.760	38.960	25.132	1.00 36.27
47										
	ATOM	3882	0	GLN			76.448	39.117	26.317	1.00 37.04
	MOTA	3883	СВ	GLN			79.101	38.277	25.861	1.00 36.81
	ATOM	3884	CG	GLN	Α	508	80.602	38.172	25.575	1.00 36.67
	ATOM	3885	CD	GLN			81.371	37.494	26.673	1.00 34.39
50	ATOM	3886		GLN			82.271	38.098	27.272	1.00 37.16
50	ATOM	3887		GLN			81.082	36.222	26.906	1.00 32.55
										1.00 35.31
	ATOM	3888	N	MET			75.851	38.873	24.172	
	MOTA	3889	CA	MET			74.428	39.078	24.429	1.00 35.41
	ATOM	3890	С	MET	Α	509	73.742	37.843	24.986	1.00 34.31
55	MOTA	3891	0	MET	Α	509	74.036	36.754	24.543	1.00 33.81
	ATOM	3892	СВ	MET			73.741	39.499	23.125	1.00 35.57
	ATOM	3893	CG	MET			74.126	40.891	22.688	1.00 38.49
	ATOM	3894	SD	MET		_	73.589	42.110	23.958	1.00 44.97
	MOTA	3895	CE	MET			71.763	41.920	23.553	1.00 40.97
60	MOTA	3896	N	PRO	Α	510	72.811	38.009	25.935	1.00 33.30
	ATOM	3897	CA	PRO			72.090	36.869	26.499	1.00 33.10
	ATOM	3898	C.	PRO			71.177	36.307	25.465	1.00 33.21
	MOTA	3899	0	PRO			70.964	36.980	24.485	1.00 32.54
	MOTA	3900	CB	PRO			71.163	37.501	27.580	1.00 33.42
65	ATOM	3901	CG	PRO	Α	510	71.103	38.917	27.314	1.00 32.83
	MOTA	3902	CD	PRO			72.326	39.288	26.467	1.00 32.45
	ATOM	3903	N	SER			70.589	35.145	25.706	1.00 33.60
	MOTA	3904	CA	SER			69.579	34.638	24.807	1.00 34.17
	MOTA	3905	Ċ	SER			68.271	34.653	25.565	1.00 34.99
70	ATOM	3906	0	SER	Α	511	68.233	34.799	26.804	1.00 34.35

	ATOM			SER A 511		69.86	4 33.20	1 24.375	7 1.00 34.66
	ATOM ATOM	_		SER A 511		69.992	2 32.34	5 25.508	3 1.00 34.37
	ATOM		N CA	LYS A 512 LYS A 512		67.201 65.893			
	5 ATOM	3911	C	LYS A 512		65.214			
	ATOM	_	0	LYS A 512		65.164	1 32.71	23.866	1.00 32.89
	ATOM ATOM		CB CG	LYS A 512 LYS A 512		65.107			
	ATOM		CD	LYS A 512		63.673 63.040			
10			CE	LYS A 512		61.708			
	ATOM ATOM		NZ	LYS A 512		61.085	38.350	24.967	
	ATOM	3918 3919	N CA	LYS A 513 LYS A 513		64.699			
	ATOM	3920	C	LYS A 513		63.992 62.537	31.219 31.497		
15		3921	0	LYS A 513		62.257	32.062		
	ATOM ATOM	3922 3923	CB CG	LYS A 513 LYS A 513		64.575		26.889	1.00 35.33
	ATOM	3924	CD	LYS A 513		64.510 63.413			
20	ATOM	3925	CE	LYS A 513		63.589		26.788	
20	ATOM ATOM	3926 3927	NZ	LYS A 513		64.157	25.601	27.953	1.00 45.70
	ATOM	3928	N CA	LEU A 514 LEU A 514		61.621 60.191			1.00 34.65
	ATOM	3929	C	LEU A 514		59.563	31.352 29.987		1.00 34.56 1.00 35.35
25	ATOM	3930	0_	LEU A 514		59.745			1.00 33.33
25	ATOM ATOM	3931 3932	CB CG	LEU A 514 LEU A 514		59.676	32.293	24.396	1.00 34.74
	ATOM	3933		LEU A 514		58.176 57.816	32.603 33.292	24.293	1.00 34.11
	ATOM	3934	CD2	LEU A 514		57.357	31.351	23.019 24.362	1.00 32.68 1.00 35.00
30	ATOM ATOM	. 3935 3936	N	ASP A 515		58.784	29.555	26.374	1.00 36.47
50	ATOM	3937	CA	ASP A 515 ASP A 515		58.292 57.200	28.194 28.147	26.393	
	MOTA	3938	ō	ASP A 515		56.814	29.193	27.455 27.991	1.00 38.11 1.00 38.35
	ATOM	3939	CB	ASP A 515		59.456	27.286	26.789	1.00 38.33
35	ATOM ATOM	3940 3941	CG OD1	ASP A 515 ASP A 515		59.343	25.856	26.271	1.00 39.55
	ATOM	3942	OD2	ASP A 515		58.247 60.367	25.307 25.168	26.003 26.131	1.00 40.04 1.00 46.00
	ATOM	3943	N	PHE A 516		56.757	26.944	27.796	1.00 46.00
	ATOM ATOM	3944 3945	CA C	PHE A 516 PHE A 516		55.673	26.763	28.721	1.00 39.35
40	ATOM	3946		PHE A 516		55.867 56.629	25.545 24.643	29.646 29.343	1.00 40.21
	ATOM	3947	CB	PHE A 516		54.363	26.612	27.924	1.00 40.04 1.00 39.53
	ATOM ATOM	3948 3949	CG	PHE A 516 PHE A 516		54.296	25.371	27.028	1.00 39.01
	ATOM	3950	CD2	PHE A 516		53.835 54.612	24.148 25.451	27.536	1.00 41.98
45	ATOM	3951	CE1	PHE A 516		53.735	23.431	25.677 26.707	1.00 39.54 1.00 41.97
	ATOM ATOM	3952 3953	CE2	PHE A 516		54.510	24.324	24.817	1.00 40.66
	ATOM		CZ N	PHE A 516 ILE A 517		54.072 55.183	23.102 25.561	25.331	1.00 41.88
	ATOM	3955	CA	ILE A 517		55.081	24.403	30.777 31.646	1.00 41.13 1.00 42.46
50	ATOM			ILE A 517		53.589	24.075	31.754	1.00 42.46
	ATOM ATOM		O CB	ILE A 517 ILE A 517		52.729	24.922	31.461	1.00 43.22
	ATOM		CG1	ILE A 517		55.692 54.909	24.669 25.757	33.035 33.752	1.00 42.62
	ATOM	3960	CG2	ILE A 517		57.195	25.002	32.910	1.00 43.03 1.00 42.66
55	ATOM ATOM		CD1	ILE A 517		55.637	26.398	34.873	1.00 43.74
	ATOM		N : CA :	ILE A 518 ILE A 518		53.285 51.915	22.846 22.378	32.155	1.00 45.38
	MOTA	3964	C :	ILE A 518		51.552	22.378	32.232 33.670	1.00 47.13 1.00 48.18
60	ATOM		0 1	ILE A 518	•	52.152	21.424	34.374	1.00 48.20
00	ATOM ATOM		CB]	LE A 518 LE A 518		51.776	21.025	31.508	1.00 47.75
	ATOM		CG2 1	LE A 518		51.830 50.454	21.240 20.360	30.010 31.843	1.00 48.10
	ATOM	3969 (CD1 1	LE A 518		51.486	19.994	29.206	1.00 47.35 1.00 49.90
65	ATOM ATOM			EU A 519		50.574	22.983	34.133	1.00 49.54
33	ATOM			EU A 519 EU A 519		50.291 49.224	22.939 21.931	35.565	1.00 50.67
	ATOM	3973 (O L	EU A 519		49.224	20.850	35.914 36.438	1.00 51.47 1.00 52.15
	ATOM		CB L	EU A 519		50.001	24.321	36.129	1.00 52.15
70	ATOM ATOM		CG L	EU A 519 EU A 519		51.301	24.933	36.671	1.00 51.17
				O Y 313		51.149	26.363	37.118	1.00 50.67

	ATOM	3977	CD2	LEU P		51.82		37.830	1.00 52.15
	ATOM	3978	N	ASN A		47.96		35.651	1.00 51.84
	ATOM	3979	CA	ASN A		46.95		35.875	1.00 52.12
5	ATOM ATOM	3980 3981	C	ASN A		46.84 47.72		34.517	1.00 51.91
,	ATOM	3982	O CB	ASN A		45.68		34.154 36.416	1.00 53.00 1.00 52.46
	ATOM	3983	CG	ASN A		45.87		37.808	1.00 53.98
	ATOM	3984		ASN A		46.29		38.728	1.00 56.71
	ATOM	3985		ASN A		45.59		37.952	1.00 57.42
10	ATOM	3986	N	GLU A		45.812		33.738	1.00 50.80
	ATOM	3987	CA	GLU A		45.83		32.357	1.00 50.22
	ATOM	3988	C	GLU A		45.979		31.510	1.00 48.04
	ATOM ATOM	3989 3990	O CB	GLU A		45.363 44.530		30.466 31.917	1.00 48.73
15	ATOM	3991	CG	GLU A		44.052		32.650	1.00 51.10 1.00 53.30
	ATOM	3992	CD	GLU A		42.569		32.365	1.00 55.46
	MOTA	3993	OE1			42.090		31.189	1.00 55.06
	ATOM	3994	OE2	GLU A	521	41.856		33.318	1.00 56.66
	ATOM	3995	N	THR A		46.779		31.948	1.00 45.52
20	MOTA	3996	CA.	THR A		46.809		31.272	1.00 43.32
	ATOM	3997	C	THR A		48.208		31.061	1.00 41.37
	ATOM ATOM	3998 3999	O CB	THR A		49.030 45.958		31.973 32.089	1.00 39.46
	ATOM	4000		THR A		44.579		32.089	1.00 43.52 1.00 44.31
25	ATOM	4001	CG2			45.954		31.432	1.00 43.41
	ATOM	4002	N	LYS A		48.439		29.851	1.00 39.61
	MOTA	4003	CA	LYS A		49.709		29.493	1.00 38.88
	ATOM	4004	C	LYS A	523	49.904		30.083	1.00 36.51
20	ATOM	4005	0	LYS A		49.067		29.929	1.00 34.48
30	ATOM ATOM	4006 4007	CB CG	LYS A		49.799		27.971 27.245	1.00 39.44
	ATOM	4007	CD	LYS A		49.762 50.100		27.245	1.00 43.67 1.00 47.88
	ATOM	4009	CE	LYS A		49.565		24.868	1.00 47.88
	ATOM	4010	NZ	LYS A		49.673		23.387	1.00 53.42
35	ATOM	4011	N	PHE A		51.032		30.746	1.00 34.85
	ATOM	4012	CA	PHE A		51.373		31.256	1.00 33.50
	ATOM	4013	C	PHE A		52.734		30.726	1.00 33.08
	ATOM ATOM	4014 4015	O CB	PHE A		53.660 51.317		30.865	1.00 34.18
40	ATOM	4015	CG	PHE A		49.951		32.750 33.268	1.00 32.45 1.00 30.56
	ATOM	4017		PHE A		49.126		33.244	1.00 30.50
	ATOM	4018		PHE A		49.474		33.785	1.00 30.79
	MOTA	4019		PHE A		47.881	29.403	33.723	1.00 30.52
	ATOM	4020		PHE A		48.182		34.289	1.00 29.32
45	ATOM	4021	CZ	PHE A		47.384		34.262	1.00 30.30
	ATOM ATOM	4022 4023	N CA	TRP A		52.846 54.031		30.104	1.00 31.67
	ATOM	4023	C	TRP A		55.013		29.376 30.236	1.00 30.71 1.00 31.46
	ATOM	4025	ŏ	TRP A		54.614		31.157	1.00 31.40
50	ATOM	4026	CB	TRP A		53.606		28.194	1.00 30.95
	MOTA	4027	CG	TRP A		52.901	30.439	27.136	1.00 28.92
	ATOM	4028		TRP A		51.590		27.110	1.00 32.14
	ATOM	4029		TRP A		53.497		25.966	1.00 32.39
55	ATOM ATOM	4030 4031		TRP A		51.330	29.328	25.975	1.00 33.71
33	ATOM	4032	CE3	TRP A		52.485 54.787	29.216 29.912	25.248 25.439	1.00 32.14 1.00 31.16
	ATOM	4033		TRP A		52.726	28.570	24.045	1.00 31.10
	ATOM	4034	CZ3	TRP A		55.016	29.271	24.217	1.00 35.24
	MOTA	4035	CH2	TRP A	525	53.984	28.624	23.541	1.00 33.52
60	MOTA	4036	N	TYR A		56.301	30.894	29.944	1.00 31.49
	ATOM	4037	CA	TYR A		57.342	31.643	30.601	1.00 31.28
	ATOM	4038	C	TYR A		58.430	31.992	29.634	1.00 31.22
	ATOM ATOM	4039 4040	O CB	TYR A		58.557 57.960	31.404	28.561	1.00 29.20
65	ATOM	4041	CG	TYR A		57.960 58.767	30.847 29.648	31.721 31.266	1.00 31.72 1.00 33.50
	ATOM	4042		TYR A		58.139	28.468	30.883	1.00 36.96
	MOTA	4043	CD2	TYR A	526	60.134	29.677	31.275	1.00 36.22
	MOTA	4044		TYR A		58.855	27.372	30.484	1.00 36.32
70	ATOM	4045		TYR A		60.882	28.576	30.878	1.00 38.01
70	MOTA	4046	CZ	TYR A	526	60.232	27.431	30.478	1.00 38.10

	ATOM ATOM ATOM ATOM 5 ATOM ATOM	4048 4049 4050 4051	N GLM CA GLM C GLM	R A 526 I A 527 I A 527 I A 527 I A 527	60.96 59.23 60.40 61.57 61.44	8 32.96° 8 33.33° 9 33.41° 4 33.834	30.046 5 29.294 7 30.234 4 31.391	1.00 31.39 1.00 30.10 1.00 30.59
10	ATOM ATOM ATOM	4053 4054 4055 4056 4057 4058	CG GLN CD GLN OE1 GLN NE2 GLN N MET CA MET	A 527 A 528 A 528	60.22 59.92 60.06 59.464 60.888 62.735	35.884 7 37.144 4 37.288 8 38.066 5 33.028 9 33.136	29.404 28.614 27.526 29.113 29.730 30.485	1.00 29.04 1.00 26.06 1.00 26.65 1.00 20.18 1.00 30.18
15	ATOM	4059 4060 4061 4062 4063 4064	O MET CB MET CG MET SD MET	A 528 A 528 A 528 A 528 A 528 A 528	64.915 65.091 64.508 63.987	33.695 31.751 31.170 29.594	28.494 30.758 31.968 32.377	1.00 31.92 1.00 31.39 1.00 32.07 1.00 32.27 1.00 36.87
20	ATOM	4065 4066 4067 4068	N ILE CA ILE C ILE O ILE	A 529 A 529 A 529 A 529 A 529 A 529	65.854 65.569 66.678 67.992 68.279 66.513	34.873 35.526 34.929 34.971	30.349 29:725 30.256 31.458	1.00 40.66 1.00 31.96 1.00 32.44 1.00 33.22 1.00 32.16
25	ATOM ATOM ATOM ATOM ATOM	4070 4071 4072 4073	CG1 ILE CG2 ILE CD1 ILE N LEU	A 529 A 529	65.543 67.834 64.917 68.765 69.910	37.355 37.722	29.784 28.620 29.522 28.695 29.333	1.00 33.33 1.00 34.42 1.00 32.58 1.00 35.57 1.00 33.52
30	ATOM ATOM ATOM ATOM ATOM	4076 4077 4078 4079	C LEU O LEU CB LEU CG LEU CD1 LEU	A 530 A 530 A 530 A 530 A 530	71.246 71.452 69.862 68.562 68.568	34.171 34.784 32.182 31.387 30.215	29.689 29.402 28.361 28.957 29.099 28.183	1.00 34.80 1.00 35.01 1.00 34.02 1.00 35.02 1.00 36.00
35	ATOM ATOM ATOM ATOM ATOM	4080 (4081 I 4082 (4083 (CD2 LEU N PRO CA PRO C PRO	A 530 A 531 A 531 A 531 A 531	68.343 72.153 73.519 74.156 73.874	30.900 34.019 34.505 33.893 32.737	30.488 30.358 30.216 28.989 28.657	1.00 38.87 1.00 37.15 1.00 35.65 1.00 36.34 1.00 37.00 1.00 36.54
40	ATOM ATOM ATOM ATOM ATOM	4086 0 4087 0 4088 N	CB PRO CG PRO CD PRO N PRO	A 531 A 531 A 531 A 532 A 532	74.219 73.102 71.903 75.065 75.736	33.979 33.815 33.399 34.615 34.112	31.475 32.504 31.665 28.370 27.172	1.00 36.87 1.00 36.79 1.00 35.99 1.00 38.89
45	ATOM ATOM ATOM ATOM ATOM	4093 C	PRO PRO DE PRO DEPENDE PRO DEPENDE PRO DE PRO DEPENDE PRO DE PRODUE PRO DE PRO	A 532 A 532 A 532 A 532 A 532	76.540 76.969 76.687 76.937 75.653	32.899 32.844 35.249 35.960 35.878	27.578 28.726 26.799 28.098	1.00 40.94 1.00 42.87 1.00 42.62 1.00 40.71 1.00 40.62
50	ATOM ATOM ATOM ATOM ATOM	4095 N 4096 C 4097 C 4098 O	HIS A A HIS A HIS A	A 533 A 533 A 533 A 533	76.762 77.589 76.869 77.483	31.956 30.799 30.036 29.434	28.850 26.671 27.004 28.093 28.973	1.00 39.14 1.00 45.30 1.00 46.60 1.00 47.82 1.00 48.86
55	ATOM ATOM ATOM ATOM ATOM	4100 C 4101 N 4102 C 4103 C	G HIS A D1 HIS A D2 HIS A E1 HIS A E2 HIS A	A 533 A 533 A 533 A 533	78.962 79.694 80.744 79.527 81.196	31.264 32.095 32.924 32.227 33.523	27.483 26.477 26.812 25.138 25.723	1.00 46.56 1.00 49.41 1.00 52.76 1.00 50.29 1.00 51.60
60	ATOM ATOM ATOM ATOM	4105 N 4106 C 4107 C 4108 O	PHE A A PHE A PHE A PHE A	534 534 534 534	80.479 75.548 74.730 75.164 75.581	33.111 30.097 29.426 27.993 27.452	24.695 28.045 29.019 29.055 28.046	1.00 51.07 1.00 48.63 1.00 48.96 1.00 50.42 1.00 50.40
65	ATOM ATOM ATOM ATOM	4112 CI 4113 CE	G PHE A D1 PHE A D2 PHE A E1 PHE A	534 534 534 534	73.264 72.362 72.208 71.681 71.388	29.510 28.767 29.175 27.654 28.498	28.629 29.551 30.859 29.117	1.00 48.57 1.00 47.33 1.00 46.58 1.00 47.50 1.00 46.08
70	ATOM ATOM ATOM	4114 CE 4115 CZ 4116 N	E2 PHE A Z PHE A ASP A	534	70.848 70.701 75.064	26.969 27.391	29.965 31.263	1.00 45.08 1.00 47.28 1.00 46.52 1.00 51.90

	ATOM	4117	CA	ASP A	535	75.465	25.969	30.334	1.00 52.77
	ATOM	4118	C	ASP A		74.546	25.238	31.320	1.00 52.89
	ATOM	4119	ŏ	ASP A		74.634	25.411	32.545	1.00 52.37
	ATOM	4120	СВ	ASP A		76.945	25.925	30.728	1.00 53.18
_						77.425	24.531	31.095	1.00 54.56
5	ATOM	4121	CG	ASP A					
	MOTA	4122		ASP A		76.631	23.564	31.033	1.00 54.82
	MOTA	4123		ASP A		78.594	24.330	31.494	1.00 55.84
	MOTA	4124	N	LYS A	536	73.669	24.415	30.762	1.00 53.04
	ATOM	4125	CA	LYS A	536	72.635	23.742	31.535	1.00 53.87
10	ATOM	4126	С	LYS A	536	73.202	22.771	32.549	1.00 53.98
	ATOM	4127	0	LYS A		72.456	22.064	33.237	1.00 53.62
	ATOM	4128	ČВ	LYS A		71.661	23.022	30.605	1.00 54.22
	ATOM	4129	CG	LYS A		72.271	21.887	29.778	1.00 57.03
		4130				71.204	21.191	28.873	
15	ATOM		CD	LYS A					
15	MOTA	4131	CE	LYS A		71.872	20.349	27.753	1.00 62.09
	MOTA	4132	NZ	LYS A		70.912	19.553	26.913	1.00 61.07
	ATOM	4133	N	SER A	537	74.526	22.740	32.628	1.00 54.14
	MOTA	4134	CA	SER A	537	75.216	21.897	33.572	1.00 54.42
	ATOM	4135	С	SER A	537	75.529	22.684	34.848	1.00 53.89
20	ATOM	4136	0	SER A	537	75.640	22.090	35.910	1.00 54.06
	ATOM	4137	ČВ	SER A		76.512	21.351	32.943	1.00 54.73
	ATOM	4138	ÖĞ	SER A		77.546	22.337	32.961	1.00 55.90
	ATOM	4139		LYS A		75.674	24.009	34.745	1.00 53.30
			N						
	ATOM	4140	CA	LYS A		75.971	24.840	35.911	1.00 52.24
25	ATOM	4141	C	LYS A		74.693	25.331	36.593	1.00 50.44
	ATOM	4142	0	LYS A		73.594	25.159	36.087	1.00 50.66
	ATOM	4143	CB	LYS A	538	76.875	26.004	35.526	1.00 53.03
	MOTA	4144	CG	LYS A	538	78.368	25.591	35.291	1.00 56.29
	ATOM	4145	CD	LYS A	538	79.214	25.570	36.598	1.00 59.62
30	ATOM	4146	CE	LYS A		80.632	24.978	36.375	1.00 61.60
-	ATOM	4147	NZ	LYS A		81.579	25.308	37.502	1.00 62.13
	ATOM	4148	N	LYS A		74.817	25.915	37.768	1.00 48.21
	MOTA	4149	CA	LYS A		73.621	26.344	38.484	1.00 46.43
	MOTA	4150	C	LYS A		73.671	27.826	38.569	1.00 43.84
35	ATOM	4151	0	LYS A		74.626	28.379	39.085	1.00 44.47
	ATOM	4152	CB	LYS A	539	73.561	25.731	39.872	1.00 46.45
	ATOM	4153	CG	LYS A	539	73.409	24.226	39.859	1.00 48.24
	ATOM	4154	CD	LYS A	539	72.651	23.732	41.073	1.00 51.70
	ATOM	4155	CE	LYS A		72.770	22.224	41.266	1.00 54.22
40	ATOM	4156	NZ	LYS A		72.715	21.841	42.745	1.00 55.81
10	ATOM	4157	N	TYR A		72.667	28.481	38.019	1.00 41.27
						72.652			1.00 41.27
	ATOM	4158	CA	TYR A			29.927	38.024	
	ATOM	4159	C	TYR A		71.631	30.452	39.038	1.00 37.60
	MOTA	4160	0	TYR A		70.668	29.765	39.412	1.00 37.20
45	ATOM	4161	CB	TYR A	540	72.319	30.444	36.636	1.00 38.62
	ATOM	4162	CG	TYR A	540	73.256	30.008	35.541	1.00 36.88
	ATOM	4163	CD1	TYR A	540	73.229	28.715	35.043	1.00 38.33
	ATOM	4164	CD2	TYR A	540	74.154		34.981	1.00 36.48
	ATOM	4165		TYR A		74.084	28.324	34.034	1.00 37.41
50	ATOM	4166		TYR A		75.007	30.526	33.998	1.00 36.38
50	ATOM	4167	CZ	TYR A		74.972	29.240	33.519	1.00 38.66
	ATOM	4168	ОН	TYR A		75.824	28.891	32.493	1.00 42.11
	ATOM	4169	N	PRO A		71.882	31.646	39.535	1.00 35.14
	ATOM	4170	CA	PRO A		70.912	32.313	40.364	1.00 34.83
55	ATOM	4171	С	PRO A	541	69.819	32.812	39.436	1.00 34.12
	ATOM	4172	0	PRO A	541	70.087	33.081	38.244	1.00 34.78
	MOTA	4173	СВ	PRO A		71.685	33.482	40.946	1.00 34.50
	ATOM	4174	CG	PRO A		72.834	33.650	40.130	1.00 34.44
	ATOM	4175	CD	PRO A		73.110	32.418	39.401	1.00 35.37
60									
60	ATOM	4176	N	LEU A		68.623	32.968	39.980	1.00 32.64
	ATOM	4177	CA	LEU A		67.495	33.359	39.177	1.00 32.09
	MOTA	4178	С	LEU A		66.729	34.491	39.834	1.00 31.18
	MOTA	4179	0	LEU A	542	66.435	34.432	41.008	1.00 31.28
	ATOM	4180	CB	LEU A	542	66.613	32.139	38.958	1.00 32.37
65	MOTA	4181	CG	LEU A		65.383	32.342	38.059	1.00 32.55
	ATOM	4182		LEU A		65.322	31.290	36.999	1.00 31.31
	ATOM	4183		LEU A		64.158	32.280	38.873	1.00 33.56
	ATOM	4184	N N	LEU A		66.479	35.536	39.052	1.00 33.30
70	ATOM	4185	CA	LEU A		65.644	36.658	39.420	1.00 28.73
70	MOTA	4186	С	LEU A	543	64.297	36.502	38.690	1.00 28.32

	ATOM	418	7 0	T.FII	A 543	64 24	C 2C 42	0 25 45	
	ATOM		_		A 543	64.240 66.27			
•	ATOM			LEU	A 543	66.028			
	АТОМ 5 АТОМ		O CI	1 LEU	A 543	66.019	9 40.46		
•	5 ATOM ATOM		S M	2 LEU	A 543 A 544	64.824			1.00 27.96
	ATOM				A 544 A 544	63.208 61.890			
	ATOM				A 544	61.387			
•	MOTA	4195			A 544	61.193			
10		4196			A 544	60.930	35.574	39.667	
	MOTA MOTA	4197 4198		LEU 1 LEU	A 544	60.008		39.230	1.00 30.70
	ATOM	4199	CD	2 LEU .	A 544 A 511	58.839 59.531	34.547		
	ATOM	4200	_	ASP .	A 545	61.145			1.00 33.99 1.00 27.80
15		4201	_	ASP .	A 545	60.688			
	ATOM ATOM	4202	_	ASP A	A 545	59.175		37.011	
	ATOM	4203 4204	-	ASP	A 545 A 545	58.687			1.00 27.66
	ATOM	4205			A 545	61.472 61.014			
20		4206	OD:	1 ASP A	A 545	60.215			1.00 29.19 1.00 34.08
	ATOM	4207		2 ASP A	A 545	61.391	41.583	34.254	
	ATOM ATOM	4208 4209			546	58.422			1.00 26.54
	ATOM	4210		VAL A		56.983 56.196	39.913		1.00 26.42
25	ATOM	4211	ŏ	VAL A		56.581	41.198 42.293		1.00 25.04 1.00 24.61
	ATOM	4212	СВ	VAL A	546	56.498	39.350		1.00 24.61 1.00 27.68
	ATOM ATOM	4213	CG1	L VAL A	546	54.993	39.144	39.152	1.00 27.49
	ATOM	4214 4215	N CG2	VAL A		57.196	38.014	39.445	1.00 29.91
30	ATOM	4216	CA	TYR A		55.064 54.117	41.041 42.110		1.00 23.69
	MOTA	4217	. C	TYR A		52.846	41.436	36.842 37.281	1.00 22.57 1.00 22.98
	ATOM	4218	0	TYR A		52.406	41.613	38.424	1.00 22.38
•	ATOM ATOM	4219 4220	CB CG	TYR A		54.052	42.699	35.441	1.00 23.31
35	ATOM	4221	CD1	TYR A TYR A		53.074 53.351	43.801	35.462	1.00 25.16
	MOTA	4222	CD2			51.763	44.984 43.607	36.153 34.939	1.00 25.12 1.00 24.22
	ATOM	4223	CE1			52.371	46.016	36.257	1.00 24.22 1.00 25.27
	ATOM ATOM	4224	CE2			50.826	44.615	35.008	1.00 24.61
40	ATOM	4225 4226	CZ OH	TYR A	547	51.115	45.787	35.667	1.00 23.64
	ATOM	4227	N	ALA A		50.117 52.265	46.657 40.636	35.763 36.385	1.00 24.55
	ATOM	4228	CA	ALA A	548	51.173	39.768	36.700	1.00 22.11 1.00 20.92
	ATOM	4229	C	ALA A		49.835	40.380	37.101	1.00 21.97
45	ATOM ATOM	4230 4231	O CB	ALA A		49.047	39.706	37.671	1.00 21.06
10	ATOM	4232	N	ALA A GLY A		51.612 49.547	38.766 41.623	37.761	1.00 21.37
	ATOM	4233	CA	GLY A		48.216	42.097	36.780 37.014	1.00 22.48 1.00 23.62
	ATOM	4234	С	GLY A	549	47.287		35.950	1.00 23.62
50	ATOM ATOM	4235 4236	0	GLY A		47.764	40.960	34.964	1.00 23.68
50	ATOM	4236	N CA	PRO A		45.979	41.659	36.160	1.00 24.27
	ATOM	4238	C	PRO A		44.918 45.109	41.212 41.623	35.243 33.781	1.00 25.13
	ATOM	4239	0	PRO A		45.328	42.799	33.463	1.00 24.88 1.00 22.84
55	ATOM	4240	CB	PRO A		43.678	41.928	35.775	1.00 25.99
33	ATOM ATOM	4241 4242	CG CD	PRO A	550	43.973	42.352	37.159	1.00 25.28
	ATOM	4243	N	PRO A	550 551	45.442 45.029	42.315 40.637	37.358	1.00 24.62
	ATOM	4244	CA	CYS A	551	45.190	40.856	32.898 31.450	1.00 26.44 1.00 27.76
60	ATOM	4245	С	CYS A	551	46.656	41.022	30.984	1.00 27.76
60	ATOM	4246	0	CYS A	551	46.934	41.154	29.798	1.00 29.90
	ATOM ATOM	4247 4248	CB SG	CYS A	551	44.397	42.083	31.040	1.00 27.76
	ATOM	4249	N	CYS A SER A		42.666 47.621	41.973	31.557	1.00 33.83
	ATOM	4250	CA	SER A		47.621	41.003 41.299	31.890 31.451	1.00 27.10
65	ATOM	4251	С	SER A	552	49.660	40.071	30.870	1.00 26.44 1.00 25.68
	ATOM	4252		SER A		49.178	38.944	30.987	1.00 23.88
	ATOM ATOM	4253 4254		SER A		49.758	41.845	32.618	1.00 26.57
	ATOM	4254		SER A GLN A		49.863 50.792	40.817	33.568	1.00 29.75
70	ATOM	4256		GLN A		51.598	40.323 39.286	30.226 29.634	1.00 25.00
							-5.200	29.034	1.00 25.59

	ATOM	4257	С	GLN	A	553	53.039	39.648	29.727	1.00	25.83
	ATOM	4258	ŏ	GLN			53.472	40.647	29.162	1.00	
	ATOM	4259	ČВ	GLN			51.244	39.143	28.159	1.00	25.82
	ATOM	4260	CG	GLN			52.067	38.059	27.375	1.00	
5	ATOM	4261	CD	GLN			51.497	37.831	25.969		24.66
,	ATOM	4262	OE1				51.699	38.647	25.100		28.01
•	ATOM	4263	NE2				50.793	36.736	25.767	1.00	22.88
	ATOM	4264	NEZ	LYS			53.795	38.812	30.418	1.00	27.54
	ATOM	4265	CA	LYS			55.215	39.028	30.609	1.00	28.83
10	ATOM	4266	C	LYS			56.100	38.043	29.838	1.00	29.25
10	ATOM	4267	Ö	LYS			57.315	38.218	29.801	1.00	29.54
	ATOM	4268	СВ	LYS			55.530	38.858	32.095	1.00	30.04
	ATOM	4269	CG	LYS			55.528	40.130	32.889	1.00	32.17
		4203		LYS			56.755	40.130	32.524	1.00	32.17
16	MOTA		CD	LYS				40.982	33.734	1.00	
15	MOTA	4271	CE				57.468				29.61
	ATOM	4272	NZ	LYS			58.540	42.527	33.279	1.00	26.97
	ATOM	4273	N	ALA			55.527	36.971	29.303	1.00	29.98
	ATOM	4274	CA	ALA			56.279	36.058	28.419	1.00	29.87
20	MOTA	4275	C	ALA			55.928	36.357	26.981	1.00	28.92
20	ATOM	4276	0	ALA			54.829	36.135	26.591	1.00	
	ATOM	4277	CB	ALA			55.908	34.628	28.717		30.59
	ATOM	4278	N	ASP			56.845	36.848	26.175	1.00	29.29
	ATOM	4279	CA	ASP			56.496	37.164	24.775	1.00	28.88
~-	MOTA	4280	C	ASP			57.712	37.131	23.885	1.00	28.69
25	MOTA	4281	0	ASP			58.808	36.879	24.369		29.50
	ATOM	4282	CB	ASP			55.814	38.516	24.700		28.24
	MOTA	4283	CG	ASP			56.709	39.646	25.081		29.28
	ATOM	4284	-	ASP	_		57.958	39.515	24.984	1.00	-
	ATOM	4285	OD2				56.227	40.762	25.408		33.08
30	ATOM	4286	N	THR			57.547	37.437	22.605	1.00	
	ATOM	4287	CA	THR			58.664	37.344	21.675		27.37
	ATOM	4288	C	THR			59.265	38.698	21.354	1.00	
	ATOM	4289	0_	THR			59.921	38.854	20.326	1.00	
	MOTA	4290	CB	THR			58.224	36.741	20.355		27.18
35	MOTA	4291		THR			57.098	37.466	19.876	1.00	
	MOTA	4292	CG2	THR			57.702	35.365	20.505	1.00	
	MOTA	4293	N	VAL			59.072	39.666		1.00	
	ATOM	4294	CA	VAL			59.628	40.993	22.018	1.00	
	ATOM	4295	С	VAL			61.123	41.105	22.381	1.00	
40	ATOM	4296	0	VAL			61.608	40.551	23.373	1.00	
	ATOM	4297	CB	VAL			58.806	42.038	22.782	1.00	
	ATOM	4298		VAL			59.372	43.437	22.654	1.00	
	ATOM	4299		VAL			57.362	42.018	22.308	1.00	
	ATOM	4300	N	PHE			61.851	41.822	21.517	1.00	27.05
45	ATOM	4301	CA	PHE			63.237	42.117	21.722	1.00	26.81
	ATOM	4302	С	PHE			63.436	43.293	22.649	1.00	26.85
	ATOM	4303	0	PHE			63.027	44.379	22.344	1.00	
	ATOM	4304	CB	PHE			63.920	42.482	20.405		26.92
	ATOM	4305	CG	PHE			65.371	42.745	20.567		28.33
50	ATOM	4306		PHE			66.240	41.694	20.770		31.89
	MOTA	4307		PHE			65.855	44.047	20.679		30.73
	MOTA	4308		PHE			67.630	41.947	20.978		34.04
	ATOM	4309		PHE			67.233	44.304	20.905		31.47
	ATOM	4310	CZ	PHE	A 5	59	68.107	43.258	21.044		31.74
55	ATOM	4311	N	ARG			64.173	43.118	23.729		27.22
	ATOM	4312	CA	ARG			64.360	44.244	24.644		28.08
	MOTA	4313	С	ARG			65.819	44.392	25.069		28.04
	ATOM	4314	0	ARG			66.505	43.423	25.237		27.21
	MOTA	4315	CB	ARG	A 5	60	63.498	44.072	25.894	1.00	28.98
60	MOTA	4316	CG	ARG	A 5	60	61.936	44.178	25.701	1.00	29.93
	MOTA	4317	CD	ARG	A 5	60	61.099	44.022	27.041		31.30
	MOTA	4318	NE	ARG	A 5	60	59.699	44.108	26.716	1.00	30.89
	MOTA	4319	CZ	ARG			58.919	43.085	26.413	1.00	31.97
	MOTA	4320		ARG	A 5	60	59.348	41.814	26.465	1.00	30.16
65	ATOM	4321	NH2	ARG	A 5	60	57.679	43.349	26.051	1.00	30.62
	ATOM	4322	N	LEU	A 5	61	66.271	45.632	25.207	1.00	28.54
	MOTA	4323	CA	LEU	A 5	61	67.570	45.931	25.806		28.49
	MOTA	4324	С	LEU	A 5	61	67.253	46.660	27.118		27.77
	ATOM	4325	0	LEU	A 5	61	66.930	47.867	27.145		26.56
70	MOTA	4326	СВ	LEU			68.402	46.835	24.924		28.27

5	ATOM	4327 4328 4329 4330 4331 4332	CD1 CD2 N CA C	LEU LEU ASN ASN ASN	A 561 A 561 A 562 A 562 A 562		68.919 69.466 69.999 67.359 66.937	47.274 45.183 45.935 46.508 46.000	22.684 23.927 28.212 29.482 30.646	1.00 1.00 1.00 1.00	30.62 30.40 29.88 26.75 26.54 25.75
10	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	4333 4334 4335 4336 4337 4338 4339	CB CG OD1 ND2 N	ASN ASN ASN ASN TRP	A 562 A 562 A 562 A 562 A 563 A 563		68.890 65.450 65.165 66.089 63.884 67.379	46.218 44.728 43.920 44.361 46.230	29.655 29.713 29.842 29.627 31.884	1.00 1.00 1.00 1.00	24.65 26.84 27.06 23.61 26.04 24.68
15	ATOM ATOM ATOM ATOM ATOM	4340 4341 4342 4343 4344	C 1 O 1 CB 1 CG 1	TRP TRP TRP TRP	A 563 A 563 A 563 A 563 A 563		68.154 68.391 69.484 67.428 68.183 69.474	44.332 43.859 46.310 46.093	33.063 33.121 33.452 34.321 35.607 35.897	1.00 1.00 1.00 1.00	24.77 25.75 23.51 24.44 24.88 25.62
20	MOTA MOTA ATOM MOTA MOTA	4345 4346 4347 4348	CD2 7 NE1 7 CE2 7 CE3 7	RP RP RP RP	A 563 A 563 A 563 A 563		67.652 69.770 68.665 66.390	45.528 46.121 45.554 45.038	36.800 37.202 37.773 37.159	1.00 1.00 1.00 1.00	22.46 24.87 23.96 23.58
25	ATOM ATOM ATOM ATOM	4349 4350 4351 4352 4353	CZ3 7 CH2 7 N A	RP . RP . LA .	A 563 A 563 A 563 A 564 A 564		68.475 66.213 67.245 67.343 67.496	45.061 44.541 44.559 43.567 42.122	39.064 38.417 39.362 32.846 32.730	1.00 1.00 1.00	25.00 22.02 21.67 26.67 28.06
30	ATOM ATOM ATOM ATOM ATOM	4354 4355 4356 4357 4358	O A CB A N T	LA A	A 564 A 564 A 564 A 565 A 565		68.614 69.345 66.158 68.770 69.811	41.771 40.782 41.476 42.592 42.339	31.714 31.882 32.294 30.685 29.683	1.00 1.00 1.00 1.00	28.72 28.25 28.63 29.69 30.16
35	ATOM ATOM ATOM ATOM ATOM	4359 4360 4361 4362 4363	C TO	HR A HR A HR A	A 565 A 565 A 565 A 565 A 565		71.167 71.984 69.786 68.577	42.353 41.421 43.408 43.308	30.409 30.272 28.561 27.825	1.00 1.00 1.00	30.65 30.39 30.79 29.29
40	ATOM ATOM ATOM ATOM ATOM	4364 4365 4366 4367 4368	N T CA T C T O T	YR A YR A YR A YR A	A 566 A 566 A 566 A 566 A 566	-	70.853 71.387 72.617 72.833 73.909	43.135 43.401 43.541 42.434 41.869	27.490 31.190 31.963 32.971 33.032	1.00 1.00 1.00 1.00	30.55 30.73 30.63 30.91
45	ATOM ATOM ATOM ATOM ATOM	4369 4370 4371 4372 4373	CG T CD1 T CD2 T CE1 T	YR A YR A YR A YR A	A 566 A 566 A 566 A 566 A 566		72.681 73.394 74.779 72.685 75.412 73.286	44.910 44.888 44.595 45.143 44.568 45.138	32.660 34.001 34.106 35.166 35.345 36.393	1.00 1.00 1.00 1.00	31.09 31.58 31.02 28.78
50	ATOM ATOM ATOM ATOM ATOM	4374 4375 4376 4377 4378	CZ T OH T N L CA L	YR A YR A EU A EU A	566 566 567 567		74.642 75.193 71.825 71.937 72.382	44.849 44.877 42.130 41.081	36.493 37.735 33.775 34.782	1.00 1.00 1.00 1.00	30.72 25.46 30.20 29.05
55	ATOM ATOM ATOM ATOM ATOM	4379 4380 4381 4382 4383	O LI	EU A EU A EU A	567 567 567 567		73.157 70.582 70.233 68.905 71.305	39.749 38.957 40.904 42.068 41.852 42.331	34.170 34.758 35.473 36.424 37.092 37.526	1.00 1 1.00 1 1.00 1 1.00 1	28.19 28.13 27.20 25.37
60	ATOM ATOM ATOM ATOM ATOM	4384 4385 4386 4387 4388	CA AI C AI O AI	A A A A	568 568 568 568 568		71.823 72.149 73.547 74.336 71.083	39.465 38.232 38.312 37.417 37.882	33.004 32.334 31.721 31.925 31.288	1.00 3	30.10 29.91 29.69 29.40
65	ATOM ATOM ATOM ATOM ATOM	4389 4390 4391 4392 4393	N SECA SECO SECO	R A R A R A	569 569 569 569 569		73.888 75.130 76.370 77.354 75.062	39.405 39.433 39.652 39.000	31.053 30.266 31.096 30.873	1.00 3 1.00 3 1.00 3	30.36 30.98 31.60 31.24
70	ATOM ATOM ATOM	4394 4395 4396	OG SE	R A	569 570 570		76.343 76.308 77.428	40.484 40.827 40.573 40.830	29.180 28.698 32.054 32.929	1.00 2	1.57

	ATOM	4397	С	THR A 57	70	77.448	40.013	34.226	1.00	31.26
	ATOM	4398	ō	THR A 5		78.502	39.507	34.588		31.27
	ATOM	4399	CB	THR A 57	70	77.469	42.292	33.327	1.00	31.50
	ATOM	4400	OG1			77.579	43.136	32.170	1.00	28.62
5	MOTA	4401	CG2			78.754	42.568	34.151		33.70
	ATOM	4402	N	GLU A 57		76.311	39.873	34.926		30.73
	ATOM	4403	CA	GLU A 57		76.299	39.189	36.216		29.94
	ATOM	4404	C	GLU A 57	_	75.955	37.733	36.172		30.81
	ATOM	4405	0	GLU A 57		76.038	37.043	37.190		31.01
10	ATOM	4406	CB	GLU A 57		75.343	39.876	37.187		29.77
	ATOM	4407	CG	GLU A 57		75.566	41.362	37.397		30.28
	ATOM	4408	CD	GLU A 57		76.980	41.725	37.807		31.41
	MOTA	4409		GLU A 57		77.675	40.823 42.920	38.285 37.677		30.55
15	MOTA	4410 4411		GLU A 57		77.371 75.536	37.230	35.013		30.19 31.60
15	ATOM ATOM	4412	N CA	ASN A 57		75.242	35.815	34.903		30.95
	ATOM	4413	C	ASN A 57		74.082	35.378	35.749		29.28
	ATOM	4414	Õ	ASN A 57		74.063	34.293	36.321		28.59
	ATOM	4415	ČВ	ASN A 57		76.479	35.003	35.238		32.51
20	ATOM	4416	ĊĠ	ASN A 57		77.530	35.092	34.159	1.00	
	ATOM	4417		ASN A 57		77.243	34.856	32.986		41.33
	ATOM	4418		ASN A 57		78.753	35.470		1.00	40.87
	ATOM	4419	N	ILE A 57	73	73.068	36.223	35.792	1.00	28.23
	MOTA	4420	CA	ILE A 57		71.842	35.885	36.463	1.00	27.13
25	ATOM	4421	С	ILE A 57	73	70.791	35.515	35.405	1.00	27.67
	ATOM	4422	0	ILE A 57		70.650	36.199	34.423		26.39
	ATOM	4423	CB	ILE A 57		71.390	37.108	37.262		27.08
	ATOM	4424		ILE A 57	-	72.377	37.423	38.395		27.09
	ATOM	4425	CG2	ILE A 57		70.028	36.899	37.835		27.15
30	ATOM	4426	CD1	ILE A 57		72.341	38.882	38.866		25.44
	MOTA	4427	N	ILE A 57	4	70.039	34.442	35.617		28.39
	ATOM	4428	CA	ILE A 57		68.933	34.131	34.744		29.05
	ATOM	4429	C	ILE A 57		67.765	35.024	35.172		29.34 29.44
35	ATOM ATOM	4430 4431	O CB	ILE A 57 ILE A 57		67.456 68.522	35.119 32.663	36.363 34.893		28.69
33	ATOM	4431		ILE A 57		69.543	31.741	34,226		31.22
	ATOM	4432	CG2	ILE A 57		67.198	32.456	34.291		28.04
	ATOM	4434		ILE A 57		69.232	30.289	34.468		32.74
	ATOM	4435	N	VAL A 57		67.112	35.667	34.216		29.53
40	ATOM	4436	CA	VAL A 57		65.965	36.483	34.548		29.76
	ATOM	4437	C	VAL A 57		64.707	35.903	33.932		29.95
	ATOM	4438	Ō	VAL A 57		64.543	35.898	32.711		29.63
	ATOM	4439	CB	VAL A 57	'5	66.160	37.860	34.098		29.91
	MOTA	4440		VAL A 57		64.879	38.687	34.402		31.25
45	ATOM	4441		VAL A 57		67.391	38.441	34.821		29.45
	ATOM	4442	N	ALA A 57	-	63.813	35.409	34.780		28.39
	ATOM	4443	CA	ALA A 57		62.617	34.777	34.288		28.29
	ATOM	4444		ALA A 57		61.318				
50	ATOM	4445	0	ALA A 57		61.207	36.161	35.676		27.41
50	ATOM ATOM	4446	CB	ALA A 57 SER A 57		62.559 60.340	33.389 35.324	34.810 33.745		29.28 27.14
	ATOM	4447 4448	N CA	SER A 57		58.982	35.797	33.745		27.54
	ATOM	4449	CA	SER A 57		57.993	34.732	33.539		27.49
	ATOM	4450	ŏ	SER A 57		58.283	33.898	32.696		28.59
55	ATOM	4451	СВ	SER A 57		58.714	37.075	33.240	1.00	27.19
	ATOM	4452	0G	SER A 57		59.805	37.939	33.396		29.78
	ATOM	4453	N	PHE A 57		56.832	34.788	34.162		27.77
	ATOM	4454	CA	PHE A 57		55.822	33.771	34.094		28.34
	ATOM	4455	C	PHE A 57		54.423	34.359	34.048		28.40
60	ATOM	4456	0	PHE A 57		54.080	35.247	34.838	1.00	27.15
	MOTA	4457	СВ	PHE A 57		55.908	32.933	35.361		28.57
	MOTA	4458	CG	PHE A 57		54.948	31.793	35.386		29.13
	MOTA	4459		PHE A 57	8 !	55.138	30.712	34.551		33.36
	MOTA	4460		PHE A 57		53.870	31.787	36.237	1.00	27.73
65	MOTA	4461		PHE A 57		54.263	29.647	34.562		31.73
	MOTA	4462	CE2	PHE A 57		53.023	30.741	36.270		28.38
	MOTA	4463	CZ	PHE A 57		53.208	29.666	35.431		29.75
	ATOM	4464	N	ASP A 57		53.628	33.838	33.125		28.25
	ATOM	4465	CA	ASP A 57		52.275	34.249	32.922		28.24
70	MOTA	4466	С	ASP A 57	9 :	51.388	33.162	33.532	1.00	28.42

5		4467 4468 4469 4470 4471	CB CG OD1 OD2	ASP ASP ASP	A 579	52.006 52.595 52.820 52.830	32.113 34.452 35.790 36.746 36.006	31.419	1.00 28.54 1.00 30.75
10	ATOM ATOM ATOM ATOM ATOM ATOM	4472 4473 4474 4475 4476	CA C O N CA	GLY GLY GLY ARG ARG	A 580 A 580 A 580 A 580 A 581 A 581	50.018 48.557 48.182 47.710 46.301	33.399 32.489 32.909 33.736 32.384 32.769	34.771 35.469 35.376 34.523 36.267 36.224	1.00 28.17 1.00 27.52 1.00 27.45 1.00 26.73 1.00 27.25 1.00 27.30
15	ATOM ATOM ATOM ATOM ATOM ATOM	4478 4479 4480 4481 4482 4483	C O CB CG CD NE	ARG ARG ARG ARG	A 581 A 581 A 581 A 581 A 581 A 581	46.152 46.910 45.456 45.027 44.672 45.723	34.269 34.949 32.081 30.726 29.758 29.536	36.324 37.008 37.291 36.875 37.961 38.944	1.00 27.40 1.00 27.28 1.00 27.42 1.00 28.39 1.00 28.82 1.00 30.44
20	ATOM ATOM ATOM ATOM ATOM	4484 4485 4486 4487 4488	CZ NH1 NH2 N CA	ARG A ARG A GLY	A 581 A 581 A 581 A 582 A 582	45.496 44.255 46.484 45.169 44.868	28.949 28.618 28.702 34.771 36.189	40.118 40.427 40.991 35.599 35.565	1.00 33.24 1.00 33.68 1.00 34.06 1.00 28.05 1.00 28.06
25	ATOM ATOM ATOM ATOM ATOM	4489 4490 4491 4492 4493	C N CA C	GLY A SER A	A 582 A 582 A 583 A 583 A 583	45.539 45.218 46.501 47.200 46.268	36.827 37.945 36.129 36.668 36.722	34.385 34.012 33.811 32.668 31.399	1.00 27.42 1.00 28.10 1.00 26.84 1.00 26.81 1.00 26.26
30	ATOM ATOM ATOM ATOM ATOM	4494 4495 4496 4497 4498	O CB OG N CA	SER A SER A SER A GLY A	583 583 584	45.216 48.528 48.377 46.646 45.786	36.137 35.928 34.539 37.482 37.695	31.365 32.455 32.175 30.401 29.276	1.00 25.67 1.00 26.87 1.00 28.61 1.00 26.14 1.00 26.40
35	ATOM ATOM ATOM ATOM ATOM	4499 4500 4501 4502 4503	C O N CA C	GLY A GLY A TYR A TYR A	584 584 585 585	46.104 47.047 45.233 45.369 45.317	36.962 36.179 37.221 36.756 35.258	28.016 27.922 27.057 25.692 25.520	1.00 26.15 1.00 24.92 1.00 27.27 1.00 27.73 1.00 28.58
40	ATOM ATOM ATOM ATOM ATOM	4504 4505 4506 4507 4508	O CB CG CD1 CD2	TYR A	585 585 585 585	45.689 46.671 46.852 45.971 47.837	34.777 37.242 38.704 39.574 39.221	24.463 25.075 25.203 24.589 26.028	1.00 29.54 1.00 28.47 1.00 27.03 1.00 26.76 1.00 22.71
45	ATOM ATOM ATOM ATOM ATOM	4509 4510 4511 4512 4513	CE1 CE2 CZ OH N	TYR A TYR A TYR A TYR A GLN A	585 585 585 585	46.085 47.969 47.103 47.229 44.822	40.922 40.585 41.424 42.752 34.533	24.731 26.195 25.539 25.675 26.509	1.00 24.58 1.00 23.53 1.00 25.17 1.00 27.86 1.00 27.92
50	ATOM ATOM ATOM ATOM ATOM	4514 4515 4516 4517 4518	CA C O CB	GLN A GLN A GLN A GLN A	586 586 586 586			26.421 26.790 27.118 27.387 27.212	
55	ATOM ATOM ATOM ATOM ATOM	4519 4520 4521 4522 4523	CD OE1 NE2 N	GLN A GLN A GLY A GLY A	586 586 586 587	47.976 48.152 48.376 42.357	32.807 33.833 31.650 33.539 33.202	28.537 29.182 28.952 26.778 27.070	1.00 26.67 1.00 30.99 1.00 24.71 1.00 27.74 1.00 27.65
60	ATOM ATOM ATOM ATOM ATOM	4524 4525 4526 4527 4528	C O N CA	GLY A GLY A ASP A ASP A ASP A	587 587 588 588	40.580 41.413 39.281 38.717	33.584 33.852 33.622 34.063 33.097	28.491 29.356 28.719 29.985 31.115	1.00 27.30 1.00 26.71 1.00 28.24 1.00 28.72
65	ATOM ATOM ATOM ATOM ATOM	4529 4530 4531 4532 4533	O CB CG OD1	ASP A ASP A ASP A ASP A ASP A	588 588 588 588	38.938 37.258 37.048 38.045	33.493 34.378 35.713 36.441 36.115	32.288 29.804 29.127 28.955 28.737	1.00 29.23 1.00 27.88 1.00 28.82 1.00 30.71 1.00 32.40 1.00 33.98
70	MOTA MOTA MOTA	4534 4535 4536	N CA	LYS A LYS A LYS A	589 589	39.025 39.165	31.821 30.856 31.239	30.794 31.863 32.688	1.00 33.96 1.00 30.05 1.00 31.24 1.00 30.44

	ATOM	4537	0			589	40.379	31.182	33.918		30.91
	MOTA	4538	CB			589	39.336	29.435	31.333		31.78
	ATOM	4539	CG			589	39.665	28.450	32.480		36.61
-	ATOM	4540	CD			589	39.570	26.997	32.065		42.76
5	ATOM ATOM	4541 4542	CE NZ	LYS LYS			40.168 40.138	26.045 24.612	33.132 32.636		45.94 46.76
	ATOM	4543	N			590	41.473	31.583	32.008	1.00	
	ATOM	4544	CA			590	42.690	31.983	32.699	1.00	
	ATOM	4545	C			590	42.582	33.424	33.202		28.20
10	ATOM	4546	Ö			590	42.932	33.708	34.352	1.00	
	MOTA	4547	CB	ILE			43.917	31.792	31.766	1.00	29.03
	ATOM	4548	CG1				44.305	30.299	31.697		29.00
	ATOM	4549	CG2				45.086	32.594	32.253		29.24
	ATOM	4550		ILE			45.365	29.961	30.622		27.13
15	ATOM	4551 4552	N	MET MET			42.064 42.012	34.320 35.746	32.370 32.692		28.36 28.67
	ATOM ATOM	4553	CA C	MET			42.012	36.094	33.837		29.62
	ATOM	4554	Ö	MET			41.422	36.927	34.660		30.74
	ATOM	4555	ČВ	MET			41.635	36.608	31.503		28.91
20	ATOM	4556	CG			591	41.965	38.046	31.699		29.05
	MOTA	4557	SD	MET			41.724	39.127	30.289	1.00	33.19
	MOTA	4558	CE			591	39.938	39.178	30.224		33.59
	ATOM	4559	N	HIS			39.926	35.430	33.923		29.45
25	ATOM	4560	CA	HIS			38.938	35.742	34.924		29.13
25	ATOM	4561 4562	C	HIS HIS			39.151	34.959	36.190		29.85
	ATOM ATOM	4562	O CB			592	38.400 37.544	35.120 35.387	37.141 34.417		29.65 29.01
	ATOM	4564	CG	HIS			37.013	36.312	33.371		28.57
	ATOM	4565				592	37.575	37.539	33.089		29.42
30	ATOM	4566		HIS			35.917	36.216	32.593		27.96
	ATOM	4567	CE1	HIS	Α	592	36.884	38.128	32.138	1.00	27.95
	ATOM	4568	NE2	HIS			35.857	37.352	31.834		29.38
	MOTA	4569	N	ALA			40.165	34.119	36.235		29.91
25	ATOM	4570	CA	ALA			40.334	33.249	37.411		30.74
35	ATOM	4571	C	ALA			40.597	34.076	38.670		31.49
	ATOM ATOM	4572 4573	O CB	ALA ALA			40.406 41.460	33.618 32.329	39.800 37.171		31.13
	ATOM	4574	N	ILE			41.007	35.316	38.455		31.17
	ATOM	4575	CA	ILE			41.370	36.177	39.556		31.77
40	ATOM	4576	C	ILE			40.275	37.221	39.868		30.82
	ATOM	4577	0	ILE			40.446	38.085	40.734		30.47
	MOTA	4578	CB	ILE			42.747	36.727	39.206		31.82
	MOTA	4579	CG1				43.681	36.422	40.307		33.46
45	MOTA	4580	CG2	ILE			42.739	38.166	38.748		34.20
45	ATOM ATOM	4581 4582		ILE ASN		594 595	44.217 39.133	35.074	40.182 39.192		34.34 29.75
	ATOM	4583	N CA	ASN			37.991	37.079 37.952	39.192		29.75
	ATOM	4584	C	ASN			37.646	38.132	40.897		29.97
	ATOM	4585	ŏ	ASN	A	595	37.551	37.160	41.639		28.99
50	MOTA	4586	CB	ASN			36.750	37.415	38.678		29.57
	MOTA	4587	CG	ASN	Α	595	35.624	38.427	38.684	1.00	28.63
	MOTA	4588		ASN			35.857	39.582	38.438		25.10
	ATOM	4589	ND2				34.417	38.002	38.992		27.23
	ATOM	4590	N	ARG			37.467	39.373	41.327		30.19
55	ATOM ATOM	4591 4592	CA C	ARG ARG			37.202 38.201	39.666 39.018	42.735 43.710		31.75 31.80
	ATOM	4593	Õ	ARG			37.976	39.016	44.923		30.98
	ATOM	4594	ČВ	ARG .			35.733	39.305	43.130		32.08
	ATOM	4595	CG	ARG			34.696	40.340	42.630		35.72
60	ATOM	4596	CD	ARG .	A	596	33.177	39.894	42.698		41.54
	ATOM	4597	NE	ARG .			32.405	40.460	43.834	1.00	42.59
	ATOM	4598	CZ	ARG .			32.269	39.861	45.022		47.28
	ATOM	4599		ARG .			32.856	38.689	45.258		51.26
<i>(</i> =	MOTA	4600		ARG .			31.549	40.416	45.982		46.20
65	ATOM	4601	N	ARG .			39.305	38.479	43.207		31.81
	ATOM ATOM	4602 4603	CA C	ARG .			40.270 41.699	37.827 38.280	44.073 43.789		32.75 31.55
	ATOM	4604	0	ARG .			42.568	37.437	43.789		30.88
	ATOM	4605	СВ	ARG .			40.298	36.325	43.808		34.17
70	ATOM	4606	ĊĠ	ARG .			39.136	35.511	44.204		39.92
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	ATOM ATOM ATOM	4607 4608 4609	NE A	RG .	A 597 A 597 A 597	3	19.324 18.700 19.353	33.034	44.551	1.00	
5	ATOM ATOM ATOM ATOM	4610 4611 4612 4613	NH2 A N L	RG EU	A 597 A 597 A 598 A 598	4 3 4	0.672 8.677 1.967	32.474 31.412 39.573	45.688 46.168 43.672	1.00 1.00 1.00	57.37 59.75 31.19
10	ATOM ATOM	4614 4615 4616 4617	C L O L CB L	EU . EU .	A 598 A 598 A 598	4 4 4	4.165 3.700 3.461	39.573 39.597 41.481	44.553 45.687 43.174	1.00 1.00 1.00	28.97 28.81 30.07
15	ATOM ATOM ATOM	4618 4619 4620	CD1 L CD2 L N G	EU A	A 598 A 599	4 4 4	2.638 2.995 2.834 5.382	43.563 41.359 39.146	42.067 41.972 40.724 44.271	1.00 1.00 1.00	29.68 31.70 28.60
15	ATOM ATOM ATOM ATOM	4621 4622 4623 4624	C G: O G: N T:	LY A	A 599 A 599 A 599 A 600	4 4	6.314 6.217 6.696 5.586	37.315 36.919	45.309 45.727 46.802 44.903		27.10
20	ATOM ATOM ATOM ATOM	4625 4626 4627 4628	C TI	IR A	A 600 A 600 A 600	4 4	5.567 6.324 7.555 4.148	34.265 34.112	45.253 44.229 44.330 45.464	1.00 1.00 1.00	27.97 28.18 28.50
25	ATOM ATOM ATOM ATOM	4629 4630 4631 4632	N PI	IR A	A 600 A 600 A 601 A 601	4 4 4	3.360 3.461 5.603 6.192	34.878	44.315 46.601 43.247 42.293	1.00 1.00 1.00	26.47 28.89 27.45
30	ATOM MOTA ATOM MOTA	4633 4634 4635 4636	O PH CB PH CG PH	IE A IE A		4: 4:	7.363 8.336 5.132 3.997	33.381 32.689 32.249 31.581	41.488 41.225 41.343 42.005	1.00 1.00 1.00	27.67
	ATOM ATOM ATOM ATOM	4637 4638 4639 4640	CD2 PF CE1 PF	E A	601 601 601 601	42	1.191 2.706 3.127 1.642	30.643 31.884 30.049 31.268	42.999 41.633 43.604 42.218	1.00 1.00 1.00	33.45 35.26 33.70 33.26
35	ATOM ATOM ATOM ATOM	4641 4642 4643 4644	N GI CA GI	U A U A	601 602 602 602	47 48	1.852 7.310 8.419 9.676	30.355 34.654 35.256 35.166	43.202 41.137 40.392 41.258	1.00 1.00 1.00	36.32 27.82 27.51 27.74
40	ATOM ATOM ATOM ATOM	4645 4646 4647 4648	CB GL	U A U A	602 602 602 602	5 (4 8 4 8	0.784 3.095 3.289	34.902 36.702 37.798 38.130	40.760 39.939 40.972 41.774	1.00 1.00 1.00	28.48 26.94 27.51 28.08
45	ATOM ATOM ATOM ATOM	4649 4650 4651 4652	OE1 GL OE2 GL N VA CA VA	U A U A L A L A	602 602 603 603	46 46 49 50	.393 .686 .494	37.199 39.341 35.332 35.245	42.267 41.890 42.562 43.516	1.00 1.00 1.00	29.58 26.35 28.37 28.70
50	ATOM ATOM ATOM ATOM ATOM	4653 4654 4655 4656	O VA CB VA CG1 VA	LA LA LA	603 603 603	52 50 51	.096	33.806 33.523 35.787 35.695	43.640 43.361 44.906 45.939	1.00 1.00 1.00	29.00 30.16 29.48 28.54
55	ATOM ATOM ATOM ATOM	4657 4658 4659 4660 4661	CA GL	JA JA JA	604 604 604 604	50 50 51	.650 .238 .586 .249	37.230 32.897 31.481 30.915 30.060	44.762 44.061 44.169 42.919	1.00 1.00 1.00	29.58 30.18 31.60 31.34
	ATOM ATOM ATOM ATOM	4662 4663 4664 4665	CB GL	JA JA JA	604 604 604	49 48 47	.326 .700 .337	30.629 30.585 29.897	43.006 44.364 45.733 45.668	1.00 1.00 1.00	30.85 32.23 38.37 44.37
60	ATOM ATOM ATOM	4666 4667 4668	OE2 GLI N ASI CA ASI	JA PA PA	604 605 605	46 50 51	.261 .351 .782 .362	28.723 30.558 31.332 30.797	45.144 46.091 41.746 40.513	1.00 1.00 1.00	45.08 45.55 31.12 30.50
65	ATOM ATOM ATOM ATOM	4669 4670 4671 4672	O ASI CB ASI CG ASI	P A P A P A	605 605 605	53 50 49	.785 .571 .468 .164	31.271 30.559 31.123 30.325	40.283 39.716 39.334 39.357	1.00 1.00 1.00	30.00 30.11 30.77 31.53
70	MOTA MOTA MOTA	4673 4674 4675 4676	N GL	A	605 605 606	48 53	.077 .180 .136 .516	29.378 30.583 32.464 32.921	40.177 38.602 40.740 40.641		

	ATOM	4677	С	GLN	Α	606	55.396	32.053	41.538	1.00	30.06
	ATOM	4678	0	GLN	Α	606	56.483	31.648	41.155	1.00	29.24
	ATOM	4679	ČВ			606	54.645	34.403	41.028		29.22
	ATOM	4680	CG			606	54.028	35.364	40.051		28.78
_			-								
5	ATOM	4681	CD			606	54.724	35.385	38.726		28.81
	MOTA	4682	OE1	GLN	Α	606	55.950	35.570	38.649		33.30
	ATOM	4683	NE2	GLN	Α	606	53.977	35.165	37.682	1.00	23.28
	ATOM	4684	N	TLE	Α	607	54.916	31.767	42.741	1.00	31.56
	ATOM	4685	CA			607	55.651	30.919	43.672		32.01
10											
10	ATOM	4686	C			607	55.812	29.550	43.042		33.52
	ATOM	4687	0	ILE	Α	607	56.917	28.983	43.044		33.45
	ATOM	4688	CB	ILE	Α	607	54.896	30.790	45.016	1.00	32.41
	ATOM	4689	CG1	ILE	Α	607	54.992	32.075	45.834	1.00	32.46
	ATOM	4690		ILE			55.463	29.677	45.842		32.05
1 =											
15	ATOM	4691		ILE			54.085	32.086	47.054		33.73
	ATOM	4692	N	GLU			54.734	29.021	42.460		34.16
	ATOM	4693	CA	GLU	Α	608	54.821	27.694	41.843	1.00	35.73
	ATOM	4694	С	GLU	Α	608	55.761	27.695	40.616	1.00	35.46
	ATOM	4695	õ	GLU			56.487	26.736	40.398		35.66
20							53.418	27.127	41.539		36.56
20	ATOM	4696	СВ	GLU							
	ATOM	4697	CG	GLU			53.359	25.710	40.955		40.03
	ATOM	4698	CD	GLU	Α	608	53.927	24.616	41.855	1.00	44.24
	ATOM	4699	OE1	GLU	Α	608	53.808	24.703	43.100	1.00	44.37
	MOTA	4700	OE2	GLU	А	608	54.515	23.652	41.300	1.00	48.00
25	ATOM	4701	Ŋ	ALA			55.802	28.788	39.859		34.52
23											
	MOTA	4702	CA	ALA			56.667	28.828	38.693		34.51
	ATOM	4703	С	ALA	Α	609	58.149	28.716	39.114		34.13
	ATOM	4704	0	ALA	Α	609	58.961	28.006	38.469	1.00	31.78
	ATOM	4705	CB	ALA	Α	609	56.437	30.088	37.884	1.00	33.49
30	ATOM	4706	N	ALA			58.479	29.447	40.171		34.05
20		4707	CA	ALA			59.832	29.413	40.730		34.67
	ATOM										
	ATOM	4708	С	ALA			60.224	28.026	41.238		35.08
	ATOM	4709	0	ALA	Α	610	61.354	27.575	41.035	1.00	33.89
	MOTA	4710	CB	ALA	Α	610	59.988	30.448	41.822	1.00	34.17
35	ATOM	4711	N	ARG			59.298	27.339	41.883	1.00	36.94
	ATOM	4712	CA	ARG			59.574	25.963	42.292		38.63
		4713		ARG			59.873	25.104	41.068		39.64
	ATOM		C								
	ATOM	4714	0	ARG			60.775	24.276	41.108		39.08
	ATOM	4715	CB	ARG	Α	611	58.406	25.322	43.009	1.00	38.66
40	ATOM	4716	CG	ARG	Α	611	58.196	25.752	44.416	1.00	40.91
	ATOM	4717	CD	ARG			57.304	24.810	45.195		42.36
	ATOM	4718	NE	ARG			56.252	25.580	45.850		47.02
	ATOM	4719	CZ	ARG			56.222	25.897	47.134		49.37
	MOTA	4720	NH1	ARG	Α	611	57.180	25.503	47.966		51.26
45	ATOM	4721	NH2	ARG	Α	611	55.212	26.616	47.590	1.00	51.85
	ATOM	4722	N	GLN	Α	612	59.095	25.283	40.002	1.00	40.69
	ATOM	4723	CA	GLN			59.295	24.516	38.788	1.00	42.53
	ATOM	4724		GLN			60.617			1 00	43.64
			C						30.130		
	MOTA	4725	0	GLN			61.286	24.045	37.494		44.69
50	MOTA	4726	CB	GLN			58.167	24.761	37.797		42.95
	ATOM	4727	CG	GLN	Α	612	56.828	24.301	38.290	1.00	44.37
	ATOM	4728	CD	GLN	Α	612	56.468	22.960	37.723	1.00	45.58
	ATOM	4729		GLN			56.577	22.774	36.523		49.79
	ATOM	4730		GLN			56.055	22.024	38.570		46.49
55	MOTA	4731	N	PHE			61.031	26.133	38.280		44.14
	MOTA	4732	CA	PHE			62.286	26.495	37.660	1.00	44.66
	ATOM	4733	С	PHE	Α	613	63.380	25.812	38.424	1.00	46.53
	ATOM	4734	0	PHE			64.423	25.517	37.859	1.00	46.58
	ATOM	4735	СB	PHE			62.494	28.000	37.619		44.25
CO											
60	MOTA	4736	CG	PHE			61.499	28.723	36.770		42.36
	MOTA	4737		PHE			60.871	28.089	35.727		41.01
	ATOM	4738	CD2	PHE	Α	613	61.187	30.039	37.024	1.00	41.38
	ATOM	4739		PHE			59.947	28.756	34.966		42.23
~ =	ATOM	4740		PHE			60.273	30.704	36.251		41.19
65	MOTA	4741	CZ	PHE			59.652	30.063	35.227		40.85
	ATOM	4742	N	SER			63.143	25.545	39.710		48.55
	ATOM	4743	CA	SER	Α	614	64.157	24.901	40.540	1.00	50.42
	ATOM	4744	C	SER			64.372	23.447	40.118		52.01
	ATOM	4745	ŏ	SER			65.508	23.011	40.012		52.61
70		_									
70	ATOM	4746	CB	SER	A	014	63.803	25.011	42.013	1.00	50.48

5	ATOM ATOM ATOM ATOM ATOM	4747 4748 4749 4750 4751	N CA	LYS LYS LYS	A 614 A 615 A 615 A 615 A 615		63.563 63.304 63.475 64.531 65.654	22.701 21.333 21.398	39.853 39.354 38.257	1.00 53.76 1.00 54.92 1.00 55.07
10	ATOM ATOM ATOM ATOM ATOM	4752 4753 4754 4755 4756	CG CD CE	LYS LYS LYS LYS	A 615 A 615 A 615 A 615 A 615		62.185 61.109 59.904 58.582 57.504	20.765 20.315 19.747 19.712	38.754 39.739 38.949 39.737	1.00 55.28 1.00 57.19 1.00 59.39 1.00 60.46
	ATOM ATOM ATOM ATOM	4757 4758 4759 4760	N CA C	MET MET MET MET	A 616 A 616 A 616 A 616		64.154 65.052 66.436 66.666		37.124 35.989 36.593	1.00 54.41 1.00 53.94 1.00 52.94
15	ATOM ATOM ATOM ATOM ATOM	4761 4762 4763 4764 4765	CB CG SD CE N	MET . MET .	A 616 A 616 A 616 A 616 A 617		64.651 63.228 62.789 61.286 67.354	23.477 23.495 25.145 24.766	35.188 34.607 33.893 33.068	1.00 53.70 1.00 53.76 1.00 52.40 1.00 52.15
20	ATOM ATOM ATOM ATOM	4766 4767 4768 4769	CA C O N	GLY A GLY A GLY A PHE A	A 617 A 617 A 617 A 618		68.633 69.663 70.841 69.287	21.525 21.534 22.605 22.369 23.791	36.364 37.053 36.777 37.016 36.306	1.00 51.47 1.00 49.40 1.00 48.16 1.00 48.41 1.00 46.53
25	ATOM ATOM ATOM ATOM ATOM	4770 4771 4772 4773 4774	CA C O CB CG	PHE A	A 618 A 618 A 618 A 618 A 618		70.324 70.160 70.785 70.412 69.112	24.798 26.046 27.085 25.149 25.510	36.074 36.959 36.758 34.595 33.980	1.00 44.89 1.00 43.22 1.00 42.11 1.00 44.90
30	ATOM ATOM ATOM ATOM	4775 4776 4777 4778	CD1 CD2 CE1 CE2	PHE A PHE A PHE A	A 618 A 618 A 618 A 618		68.587 68.422 67.381 67.213	26.780 24.598 27.120 24.949	34.142 33.204 33.564 32.598	1.00 46.03 1.00 47.22 1.00 46.83 1.00 46.69 1.00 46.58
35	ATOM ATOM ATOM ATOM ATOM	4779 4780 4781 4782 4783	CZ N CA C	VAL A VAL A VAL A	619 619 619		66.696 69.346 69.077 69.578 69.354	26.200 25.901 26.980 26.625 25.522	32.797 37.981 38.871 40.240 40.721	1.00 47.72 1.00 41.96 1.00 41.17 1.00 40.50
40	ATOM ATOM ATOM ATOM ATOM	4784 4785 4786 4787 4788	CB CG1	VAL A VAL A VAL A ASP A	619 619 619 620		67.586 67.224 67.136 70.247 70.709	27.235 28.165 27.807 27.573 27.386	38.920 40.078 37.593 40.874	1.00 39.68 1.00 41.06 1.00 40.61 1.00 41.96 1.00 40.71
45	ATOM ATOM ATOM ATOM	4789 4790 4791 4792	C O CB CG	ASP A ASP A ASP A	620 620 620 620		69.556 69.176 71.879 72.267	27.739 28.901 28.297 28.286	42.251 43.152 43.251 42.555 44.023	1.00 41.12 1.00 40.94 1.00 40.18 1.00 41.40 1.00 42.62
50	ATOM ATOM ATOM ATOM ATOM	4793 4794 4795 4796 4797	OD1 OD2 N CA	ASP A ASP A ASN A ASN A	620 621 621		72.863 72.035 68.988 67.804 68.046	29.274 27.352 26.777 27.161 27.908	44.465 44.813 43.849 44.584 45.909	1.00 45.71 1.00 46.38 1.00 41.25 1.00 41.89 1.00 41.34
55	ATOM ATOM ATOM ATOM ATOM ATOM	4798 4799 4800 4801 4802 4803		ASN A ASN A ASN A ASN A ASN A LYS A	621 621 621 621		67.099 66.766 67.231 67.014 67.845 69.310	28.277 26.036 24.853 23.714 25.087	46.589 44.645 45.397 44.973 46.526	1.00 39.99 1.00 43.11 1.00 45.02 1.00 50.87 1.00 46.65
60	ATOM ATOM ATOM ATOM	4804 4805 4806 4807	CA C O CB	LYS A LYS A LYS A LYS A	622 622 622 622		69.589 69.584 69.594 70.965	28.208 29.069 30.538 31.442 28.750	46.227 47.385 46.948 47.777 47.995	1.00 40.43 1.00 39.96 1.00 38.41 1.00 38.04 1.00 40.47
65	ATOM ATOM ATOM ATOM ATOM ATOM	4808 4809 4810 4811 4812 4813	CD CE NZ N	LYS A LYS A LYS A LYS A ARG A ARG A	622 622 622 623		71.167 72.658 72.827 74.269 69.596	27.286 26.933 25.462 25.016 30.773	48.347 48.474 48.888 48.993 45.639	1.00 43.46 1.00 48.43 1.00 50.37 1.00 54.19 1.00 36.15
70	ATOM ATOM ATOM	4814 4815 4816	C 0	ARG A ARG A ARG A	623 623	(68.512 68.666 71.044	32.138 32.428 32.419 32.401	45.125 44.155 42.944 44.507	1.00 34.54 1.00 33.26 1.00 30.78 1.00 34.09

	ATOM	4817	CG	ARG	Α	623	72.182	32.316	45.567	1.00	32.92
	ATOM	4818	CD			623	73.528	32.690	45.050		33.79
	ATOM	4819	NE			623	74.101	31.638	44.214		34.41
	ATOM	4820	CZ			623	74.996	31.847	43.264		35.70
5	ATOM	4821	NH1			623	75.434	33.083	43.002		33.42
3		4822	NH2			623	75.469	30.810	42.572		35.07
	ATOM						67.339	32.630	44.729		32.55
	ATOM	4823	N			624			43.941		32.44
	ATOM	4824	CA			624	66.173	33.001	44.517		
	ATOM	4825	C			624	65.601	34.288			31.62
10	MOTA	4826	0			624	65.414	34.462	45.733		30.99
	ATOM	4827	CB			624	65.194	31.896	43.906		32.85
	MOTA	4828	CG1			624	65.898	30.628	43.386		34.14
	ATOM	4829		ILE			64.053	32.277	42.979		33.93
	MOTA	4830	CD1			624	64.961	29.405	43.207		36.13
15	ATOM	4831	N			625	65.415	35.240	43.638		30.01
	ATOM	4832	CA			625	64.955	36.521	44.074		28.84
	MOTA	4833	С			625	63.726	36.829	43.262		27.42
	ATOM	4834	0	ALA	Α	625	63.473	36.172	42.250	1.00	25.18
	MOTA	4835	CB	ALA	Α	625	66.014	37.558	43.807	1.00	28.63
20	MOTA	4836	N	ILE	Α	626	63.021	37.872	43.677	1.00	26.42
	ATOM	4837	CA	ILE	Α	626	61.871	38.334	42.938	1.00	26.38
	ATOM	4838	С	ILE	Α	626	61.796	39.844	42.987	1.00	25.89
	ATOM	4839	0	ILE	Α	626	62.191	40.471	43.962	1.00	25.73
	ATOM	4840	CB	ILE	Α	626	60.623	37.689	43.494	1.00	26.45
25	ATOM	4841	CG1	ILE	Α	626	59.404	38.259	42.780	1.00	27.17
	ATOM	4842	CG2			626	60.566	37.887	45.004		26.71
	ATOM	4843	CD1			626	58.192	37.452	42.992		29.50
	ATOM	4844	N			627	61.388	40.449	41.885	1.00	25.90
	ATOM	4845	CA			627	61.195	41.883	41.870		25.90
30	ATOM	4846	C			627	60.116	42.345	40.938	1.00	
-	ATOM	4847	ŏ			627	59.762	41.680	39.959		25.99
	ATOM	4848	СВ			627	62.462	42.621	41.521		25.37
	ATOM	4849	CG			627	62.614	42.982	40.096		26.40
	ATOM	4850	CD1			627	63.003	42.147	39.090		24.57
35	ATOM	4851	CD2			627	62.464	44.288	39.505		24.31
55	ATOM	4852	NE1	TRP			63.091	42.845	37.917		26.92
	ATOM	4853	CE2	TRP			62.768	44.160	38.139		24.75
	ATOM	4854	CE3	TRP			62.781	45.546	39.994		23.17
	ATOM	4855	CZ2	TRP			62.709	45.241	37.240		24.25
40	ATOM	4856	CZ3	TRP			62.051	46.630	39.131		23.08
40						627	62.350	46.473	37.744		23.04
	ATOM	4857	CH2			628			41.219		25.40
	ATOM	4858	N				59.619	43.538	40.360		24.79
	ATOM	4859	CA			628	58.606	44.090			
45	ATOM	4860	C	GLY			58.254	45.494	40.719	1.00	23.77 21.64
45	ATOM	4861	0	GLY			58.611 57.489	45.979 46.095	41.786		23.74
	ATOM	4862	N	TRP					39.816		
	MOTA	4863	CA			629	57.087	47.503	39.854		24.09
	ATOM	4864	C	TRP			55.580	47.499	39.761	1.00	23.81
	ATOM	4865	0_	TRP			55.006	46.713	39.018		23.65
50	MOTA	4866	CB	TRP	A	629	57.675	48.188	38.630		24.46
	ATOM	4867	CG	TRP			57.929	49.640	38.721		25.53
	MOTA	4868	CD1	TRP			57.010	50.618	38.921		26.25
	ATOM	4869	CD2	TRP			59.186	50.315	38.506		23.91
	MOTA	4870		TRP			57.612	51.854	38.894		25.51
55	MOTA	4871		TRP			58.952	51.692	38.636		26.50
	MOTA	4872		TRP			60.480	49.895	38.223		20.13
	ATOM	4873	CZ2	TRP			59.973	52.646	38.490	1.00	25.09
	ATOM	4874	CZ3	TRP			61.494	50.854	38.105	1.00	21.41
	ATOM	4875	CH2	TRP			61.233	52.194	38.231	1.00	21.98
60	MOTA	4876	N	SER	Α	630	54.940	48.347	40.549	1.00	23.53
	MOTA	4877	CA	SER			53.476	48.495	40.538	1.00	23.81
	MOTA	4878	C	SER			52.706	47.239	40.961	1.00	23.46
	ATOM	4879	ō	SER			52.886	46.729	42.066		24.58
	ATOM	4880	СB	SER			53.085	48.945	39.160		23.51
65	ATOM	4881	ŌĞ	SER			52.141	49.969	39.276		23.88
	ATOM	4882	N	TYR			51.875	46.707	40.087		22.70
	ATOM	4883	CA	TYR			51.241	45.474	40.384		21.81
	ATOM	4884	C	TYR			52.357	44.489	40.697		22.55
	ATOM	4885	ŏ	TYR			52.188	43.602	41.532		21.39
70	ATOM	4886	ČВ	TYR			50.377	44.993	39.196		21.65
											

	ATOM ATOM	488	8 CD1 TYR A 6	31 49.681	42.705	39.911	
5	ATOM	489 489 489	0 CE1 TYR A 6 1 CE2 TYR A 6 2 CZ TYR A 6	31 48.712 31 47.076 31 47.414	41.805 43.499	40.385	1.00 23.19 1.00 24.52
10	ATOM ATOM ATOM ATOM ATOM	4893 4894 4895 4896 4897	4 N GLYA6 5 CA GLYA6 6 C GLYA6	32 53.494 32 54.627 32 55.255		41.053 40.006 40.239 41.627 42.239	1.00 20.91 1.00 22.19 1.00 23.91 1.00 23.98
15	ATOM MOTA ATOM ATOM ATOM	4898 4899 4900 4901 4902	8 N GLY A 6: 9 CA GLY A 6: 0 C GLY A 6: 1 O GLY A 6:	55.236 55.690 33 54.733 55.158	45.145 45.393 44.715 44.081	42.130 43.496 44.492 45.488	1.00 24.94 1.00 24.92 1.00 24.75 1.00 23.82
20	ATOM ATOM ATOM ATOM	4903 4904 4905 4906	3 CA TYR A 63 4 C TYR A 63 5 O TYR A 63 5 CB TYR A 63	34 52.419 34 52.605 34 52.688	44.834 44.239 42.715 42.100 44.605	44.202 45.024 45.065 46.134 44.478	1.00 24.12 1.00 23.97 1.00 24.59 1.00 24.79 1.00 24.31
	ATOM ATOM ATOM ATOM	4907 4908 4909 4910	CD1 TYR A 63 CD2 TYR A 63 CE1 TYR A 63	34 49.889 34 49.537 34 49.141 34 48.510	43.855 44.076 42.944 43.377	45.111 46.413 44.381 46.994	1.00 23.82 1.00 22.78 1.00 21.52 1.00 22.94
25	ATOM ATOM ATOM ATOM	4911 4912 4913 4914	CZ TYR A 63 OH TYR A 63 N VAL A 63	34 47.766 34 46.713 35 52.679	42.282 42.496 41.808 42.094	44.941 46.246 46.813 43.911	1.00 22.09 1.00 22.45 1.00 23.31 1.00 24.15
30	ATOM ATOM ATOM ATOM ATOM ATOM	4915 4916 4917 4918 4919	C VAL A 63 O VAL A 63 CB VAL A 63	55 54.173 55 54.235 55 52.755	40.652 40.241 39.251 40.093	43.888 44.517 45.199 42.452	1.00 24.87 1.00 24.65 1.00 24.18 1.00 24.90
35	ATOM ATOM ATOM ATOM	4920 4921 4922 4923	CG1 VAL A 63 CG2 VAL A 63 N THR A 63 CA THR A 63 C THR A 63	5 51.345 6 55.221 6 56.512	38.613 40.283 41.004 40.709 40.657	42.426 41.965 44.284 44.864 46.361	1.00 25.11 1.00 24.65 1.00 25.12 1.00 25.36
40	ATOM ATOM ATOM ATOM	4924 4925 4926 4927	O THR A 63 CB THR A 63 OG1 THR A 63 CG2 THR A 63	6 56.873 6 57.531 6 58.035	39.736 41.829 41.606 41.791	47.028 44.459 43.126 45.315	1.00 24.77 1.00 24.50 1.00 26.95 1.00 26.06 1.00 26.91
45	ATOM ATOM ATOM ATOM ATOM	4928 4929 4930 4931 4932	N SER A 63 CA SER A 63 C SER A 63 O SER A 63 CB SER A 63	7 55.673 7 55.569 7 54.662 7 54.916 7 55.066	41.632 41.760 40.683 40.181 43.144	46.901 48.342 48.920 50.017 48.665	1.00 24.63 1.00 24.18 1.00 25.28 1.00 24.93 1.00 23.48
50	ATOM ATOM ATOM ATOM ATOM	4933 4934 4935 4936 4937	OG SER A 63' N MET A 63' CA MET A 63' C MET A 63' O MET A 63'	7 55.954 8 53.631 8 52.741 8 53.465	44.085 40.292 39.262 37.929 37.130	48.097 48.167 48.643 48.646	1.00 22.02 1.00 24.69 1.00 24.72 1.00 24.85
55	ATOM ATOM ATOM ATOM ATOM	4938 4939 4940 4941 4942	CB MET A 638 CG MET A 638 SD MET A 638 CE MET A 638 N VAL A 639	51.476 50.589 49.706 3 48.273	39.197 40.396 40.451 39.399 37.675	49.549 47.775 47.989 49.503 49.121 47.628	1.00 23.44 1.00 25.04 1.00 25.97 1.00 24.26 1.00 28.34 1.00 24.38
60	ATOM ATOM ATOM ATOM ATOM	4943 4944 4945 4946 4947	CA VAL A 639 C VAL A 639 O VAL A 639 CB VAL A 639 CG1 VAL A 639	55.119 56.196 56.373 55.908	36.483 36.492 35.522 36.344 35.246	47.614 48.717 49.392 46.272	1.00 25.85 1.00 26.46 1.00 27.64 1.00 26.72
65	ATOM ATOM ATOM ATOM ATOM	4948 4949 4950 4951 4952	CG2 VAL A 639 N LEU A 640 CA LEU A 640 C LEU A 640 O LEU A 640	54.979 56.939 57.951 57.278	36.090 37.573 37.538 37.246	46.381 45.121 48.899 49.936 51.260 52.084	1.00 26.16 1.00 27.54 1.00 27.30 1.00 28.97 1.00 30.01
70	ATOM ATOM ATOM ATOM	4953 4954 4955 4956	CB LEU A 640 CG LEU A 640 CD1 LEU A 640 CD2 LEU A 640	58.738 59.541 59.983	38.831 39.123 40.560	50.055 48.818 48.808 48.770	1.00 30.46 1.00 28.39 1.00 30.68 1.00 31.22 1.00 32.89

	ATOM ATOM ATOM	4957 4958 4959	N CA C	GLY GLY GLY	Α	641	56.060 55.335 54.415	37.755 37.561 36.363	51.445 52.683 52.781	1.00	30.64 31.58 32.11
	ATOM	4960	Ö	GLY			53.599	36.272	53.722		
5	ATOM	4961	Ň	SER			54.541	35.419	51.854		31.43
	ATOM	4962	CA	SER			53.673	34.249	51.887		30.86
	ATOM	4963	С	SER			54.255	33.136	52.764		31.44
	ATOM	4964	0	SER	Α	642	53.576	32.123	53.033		31.55
	ATOM	4965	CB	SER			53.543	33.701	50.471	1.00	30.30
10	ATOM	4966	OG	SER			54.803	33.191	50.091		28.39
	ATOM	4967	N	GLY			55.517	33.299	53.165		31.79
	ATOM	4968	CA	GLY			56.219	32.290	53.944		32.28
	ATOM	4969	Ç	GLY			56.597	31.034	53.160		32.91
15	ATOM	4970	0	GLY			56.811	29.976	53.738		32.68
15	ATOM	4971 4972	N CA	SER			56.717	31.140	51.843		33.20
	ATOM ATOM	4973	CA	SER SER			57.001 58.383	29.960 29.357	51.022 51.263		33.35 33.95
	ATOM	4974	Ö	SER			58.575	28.159	51.265		33.80
	ATOM	4975	СВ	SER			56.890	30.322	49.557		33.20
20	ATOM	4976	ÖĞ	SER			58.097	30.922	49.129		33.53
	ATOM	4977	N	GLY			59.340	30.193	51.651		33.66
	MOTA	4978	CA	GLY			60.710	29.748	51.844		33.54
	ATOM	4979	С	GLY	Α	645	61.443	29.611	50.508	1.00	33.70
	ATOM	4980	0	GLY	Α	645	62.651	29.390	50.463	1.00	32.41
25	MOTA	4981	N	VAL			60.714	29.802	49.411		33.25
	ATOM	4982	CA	VAL			61.314	29.684	48.086		33.17
	ATOM	4983	C	VAL			62.227	30.858	47.752		32.53
	ATOM	4984	0	VAL			63.240	30.663	47.099		33.19
30	ATOM ATOM	4985 4986	CB	VAL			60.226	29.583	46.990		33.15
30	ATOM	4987		VAL VAL			60.849 59.397	29.618 28.324	45.576 47.195		33.99 33.67
	ATOM	4988	N N	PHE			61.884	32.075	48.168		31.56
	ATOM	4989	CA	PHE			62.712	33.216	47.773		30.96
	ATOM	4990	C	PHE			63.624	33.734	48.881		30.94
35	ATOM	4991	ō	PHE			63.248	33.746	50.065		30.19
	ATOM	4992	CB	PHE	Α	647	61.856	34.356	47.230		30.77
	ATOM	4993	CG	PHE	Α	647	60.940	33.951	46.099	1.00	30.66
	ATOM	4994		PHE			59.737	33.315	46.354		29.51
	ATOM	4995		PHE			61.290	34.223	44.789		27.92
40	ATOM	4996	CE1				58.887	32.943	45.286		32.03
	ATOM	4997	CE2				60.466	33.866	43.755		30.57
	ATOM ATOM	4998 4999	CZ N	PHE .			59.261 64.815	33.223 34.169	43.991		27.73 30.78
	ATOM	5000	CA	LYS .			65.806	34.169	48.474 49.399		31.48
45	ATOM	5001	C	LYS			65.645	36.169	49.604		31.25
	ATOM	5002	ŏ	LYS			65.859	36.687	50.675		30.03
	ATOM	5003	СВ	LYS			67.221	34.458	48.881		32.00
	ATOM	5004	CG	LYS .				34.871	49.892		30.90
	MOTA	5005	CD	LYS .			69.674	34.331	49.513	1.00	31.40
50	MOTA	5006	CE	LYS .			70.674	34.600	50.627		31.69
	MOTA	5007	NZ	LYS A			71.597	35.694	50.288		34.00
	ATOM	5008	N	CYS			65.267	36.857	48.546	1.00	
	ATOM	5009	CA	CYS			65.195	38.300	48.597		32.89
55	ATOM ATOM	5010 5011	C	CYS			64.291	38.773	47.485	1.00	
33	ATOM	5011	O CB	CYS Z			63.949 66.594	37.991 38.878	46.601	1.00	
	ATOM	5012	SG	CYS			67.424	38.414	48.433 46.901	1.00	
	ATOM	5014	N	GLY			63.907	40.043	47.536	1.00	
	ATOM	5015	CA	GLY A			63.102	40.625	46.489	1.00	
60	ATOM	5016	C	GLY A			62.993	42.133	46.627	1.00	
	ATOM	5017	Ō	GLY Z			63.251	42.698	47.702	1.00	
	MOTA	5018	N	ILE A			62.593	42.781	45.534	1.00	
	ATOM	5019	CA	ILE A			62.516	44.223	45.489	1.00	
	MOTA	5020	С	ILE A			61.156	44.660	44.990	1.00	
65	ATOM	5021	0	ILE A			60.721	44.216	43.920	1.00	
	MOTA	5022	CB	ILE A			63.526	44.765	44.531	1.00	
	MOTA	5023	CG1	ILE A			64.910	44.190	44.820		27.69
	ATOM	5024	CG2	ILE A			63.528	46.266	44.570	1.00	
70	ATOM	5025		ILE A			65.992	44.754	43.919	1.00	
70	ATOM	5026	N	ALA A	-7	ひコム	60.529	45.576	45.726	1.00	25.42

		ATOM ATOM ATOM ATOM	5027 5028 5029 5030	C	ALA ALA	A 652 A 652 A 652	59 59	9.212 9.287 9.646	48.354	45.063 45.922	1.00	
	5	ATOM ATOM ATOM	5031 5032 5033	N CA C	VAL VAL VAL	A 653 A 653 A 653	58 58 57	3.224 3.928 3.965 7.594	45.831 47.924 49.319 49.880	46.519 43.831 43.441 43.243	1.00 1.00 1.00	23.92 23.46 23.10
	10	ATOM ATOM ATOM ATOM	5034 5035 5036 5037	CB CG1 CG2	VAL VAL VAL	A 653	59 59 61	3.831 9.806 9.927 153	49.360 49.499 50.968 48.864	42.421 42.187 41.798 42.415		
	15	ATOM ATOM ATOM ATOM ATOM	5038 5039 5040 5041 5042	CA C O	ALA ALA ALA	A 654 A 654 A 654 A 654	56 54 54	.313 .044 .883 .016	50.956 51.634 50.657 50.702	43.970 43.964 43.980 43.148	1.00 1.00 1.00 1.00	21.63
	20	ATOM ATOM ATOM ATOM ATOM	5042 5043 5044 5045 5046	CB N CA C	PRO PRO PRO	A 654 A 655 A 655 A 655	54 53 52	.930 .846 .793 .444	52.551 49.788 48.772 49.278	42.754 44.962 45.019 45.479	1.00 1.00	23.37 23.85 24.40
	20	ATOM ATOM ATOM ATOM	5047 5048 5049 5050	O CB CG CD	PRO . PRO .	A 655 A 655 A 655 A 655	54 55 55	.332 .311 .242 .787	50.249 47.794 48.635 49.731	46.245 46.052 46.918 46.087	1.00	24.57 24.95 22.29
	25	ATOM ATOM ATOM	5051 5052 5053	N CA C	VAL . VAL .	A 656 A 656 A 656	50 50 50	.397 .092 .242 .901	48.633 48.801 47.927 46.907	44.966 45.555 46.766 46.654	1.00	23.00 23.22 23.66
	30	ATOM ATOM ATOM ATOM ATOM	5054 5055 5056 5057 5058	CB CG1 CG2 N CA	VAL A VAL A SER A		47 48 49	.996 .831 .581 .708	48.248 47.830 49.280 48.314	44.633 45.408 43.637 47.928	1.00 1.00 1.00	22.68
	3 5	ATOM ATOM ATOM ATOM	5059 5060 5061 5062	C O CB OG	SER A	A 657 A 657 A 657	48 48 50	.749 .381 .314 .497	47.460 47.086 46.142 48.154 49.330	49.139 49.698 50.476 50.306	1.00	22.94
4	40	ATOM ATOM ATOM ATOM	5063 5064 5065 5066	N CA C	ARG AARG AARG A	A 658 A 658 A 658	47 45 45	.322 .960 .028	47.821 47.573 48.259 49.447	50.750 49.328 49.773 48.770	1.00	22.76 23.64 23.86
		ATOM ATOM ATOM ATOM	5067 5068 5069 5070	CB CG CD	ARG A	4 658 4 658 4 658	45. 44. 44.	.789 .450 .608	48.118 48.173 48.584	48.447 51.197 51.828 53.292	1.00 1.00 1.00	23.24 24.97 27.68 32.89
4	15	ATOM ATOM ATOM	5071 5072 5073	NE CZ NH1 NH2	ARG A	658 658 658	42. 42. 41.	. 487 . 515 . 437 . 585	48.394 49.260 50.367 48.998	54.210 54.412 53.692 55.307	$1.00 \\ 1.00$	39.23 40.71 42.58 40.26
5	50	ATOM ATOM ATOM	5074 5075 5076 5077	N CA C	TRP ATRP ATRP A	659 659 659	43. 42. 42.	032 247 364 112	47.502 47.925 49.102 49.894	48.300 47.165 47.479 46.602	1.00 1.00	22.99 22.51 22.51 21.24
5	5	ATOM ATOM ATOM ATOM ATOM ATOM	5078 5079 5080 5081 5082 5083	CD2 NE1	TRP A TRP A TRP A TRP A TRP A TRP A	659 659 659 659	43. 43. 44. 44.	505 443 805 200 761 031	46.741 45.839 44.591 46.103 44.068 44.991	46.563 45.961 46.380 44.790 45.530 44.560	1.00 1.00 1.00	22.25 21.75 21.07 19.12 20.37
6	0	ATOM ATOM ATOM ATOM	5084 5085 5086 5087	CE3 CZ2 CZ3	TRP A TRP A TRP A TRP A	659 659 659	44. 45. 45.	288 900 162 936	47.190 44.922 47.129 45.993	43.930 43.474 42.866 42.640	1.00 1.00 1.00 1.00	20.26 21.88 21.87
6	5	ATOM ATOM ATOM ATOM	5088 5089 5090 5091	N CA C	GLU A GLU A GLU A GLU A	660 660 660		981 224 084	49.279 50.461 51.714 52.827	48.738 49.126 48.900 48.778	1.00 1.00 1.00	23.00 22.39
		ATOM ATOM ATOM ATOM	5092 5093 5094 5095	CB CG CD	GLU A GLU A GLU A GLU A	660 660 660	40. 39. 39.	676 392 262	50.387 49.556 48.942 47.858	50.588 50.770 52.189	1.00 1.00 1.00	24.05 26.09 30.94
70	0	ATOM	5096		GLU A		38.		49.524	52.484 53.046	1.00	

ATOM 5099 C TYR A 661 44.228 53.126 46.967 1.00 21.3 5 ATOM 5101 CB TYR A 661 45.611 52.589 48.930 1.00 22.3 ATOM 5103 CD1 TYR A 661 45.611 52.589 48.930 1.00 22.3 ATOM 5103 CD1 TYR A 661 45.611 52.589 48.930 1.00 23.1 ATOM 5104 CD2 TYR A 661 45.611 52.589 53.014 51.351 1.00 24.4 ATOM 5105 CEI TYR A 661 46.887 51.717 50.905 1.00 21.2 ATOM 5106 CEZ TYR A 661 46.887 51.717 50.905 1.00 24.7 ATOM 5107 CZ TYR A 661 47.100 51.566 52.259 1.00 24.7 ATOM 5108 CH TYR A 661 46.28 52.117 53.144 1.00 22.0 ATOM 5108 CH TYR A 661 46.446 51.935 54.523 1.00 21.5 ATOM 5109 N TYR A 662 43.996 52.192 46.063 1.00 21.5 ATOM 5110 CA TYR A 662 44.991 52.436 44.647 1.00 21.5 ATOM 5111 C TYR A 662 44.091 52.436 44.647 1.00 22.5 ATOM 5112 C TYR A 662 44.657 51.187 43.933 1.00 22.2 ATOM 5113 CB TYR A 662 44.657 51.187 43.933 1.00 22.2 ATOM 5114 CG TYR A 662 44.657 51.187 43.933 1.00 22.2 ATOM 5115 CD1 TYR A 662 44.657 51.187 43.933 1.00 22.2 ATOM 5116 CD2 TYR A 662 44.657 51.187 43.933 1.00 22.2 ATOM 5117 CEI TYR A 662 45.229 52.581 42.568 1.00 22.7 ATOM 5118 CCZ TYR A 662 45.227 51.326 40.236 1.00 21.3 ATOM 5119 CZ TYR A 662 45.227 51.326 40.236 1.00 21.3 ATOM 5119 CZ TYR A 663 42.925 53.492 42.736 1.00 22.3 ATOM 5112 C ASP A 663 42.92 52.345 40.214 1.00 22.5 ATOM 5122 CA ASP A 663 42.92 53.492 42.736 1.00 22.3 ATOM 5122 CA ASP A 663 42.92 53.492 42.736 1.00 22.3 ATOM 5122 CA ASP A 663 42.92 53.492 42.736 1.00 22.3 ATOM 5122 CA ASP A 663 42.92 53.492 42.736 1.00 22.3 ATOM 5123 C ASP A 663 42.293 55.065 40.984 1.00 22.3 ATOM 5124 CA SPR A 663 42.293 55.065 40.984 1.00 22.3 ATOM 5125 CB ASP A 663 42.293 55.065 40.984 1.00 23.0 ATOM 5126 CG ASP A 663 42.293 55.065 40.984 1.00 23.0 ATOM 5133 C ASP A 663 42.293 55.065 40.984 1.00 23.0 ATOM 5133 C ASP A 663 42.293 55.065 40.984 1.00 23.0 ATOM 5133 C ASP A 663 42.293 55.065 40.984 1.00 23.0 ATOM 5133 C ASP A 663 42.293 55.065 40.984 1.00 23.0 ATOM 5133 C ASP A 663 42.293 55.055 40.984 1.00 23.0 ATOM 5133 C ASP A 663 42.395 54.229 39.179 1.00 24.4 ATOM 5133 C ASR A 664 37.655 38.307 52.220 41.71	398 398 3147 316 316 316 317 317 317 317 317 317 317 317 317 317
ATOM 5102 CG TYR A 661 45.819 52.433 50.422 1.00 23.1 ATOM 5103 CD1 TYR A 661 44.956 53.014 51.351 1.00 24.4 ATOM 5105 CE1 TYR A 661 46.887 51.717 50.905 1.00 21.2 ATOM 5105 CE1 TYR A 661 45.166 52.840 52.693 1.00 24.7 ATOM 5106 CE2 TYR A 661 47.100 51.566 52.259 1.00 20.6 ATOM 5107 CZ TYR A 661 46.248 52.117 53.144 1.00 22.0 ATOM 5108 OH TYR A 661 46.248 52.117 53.144 1.00 22.0 ATOM 5109 N TYR A 662 44.091 52.436 44.647 1.00 21.5 ATOM 5110 CA TYR A 662 44.091 52.436 44.647 1.00 21.5 ATOM 5111 C TYR A 662 44.091 52.436 44.647 1.00 21.5 ATOM 5111 C TYR A 662 44.091 52.436 44.697 1.00 21.5 ATOM 5112 O TYR A 662 44.657 51.187 43.933 1.00 22.2 ATOM 5113 CB TYR A 662 44.657 51.187 43.933 1.00 22.2 ATOM 5113 CB TYR A 662 44.657 51.187 43.933 1.00 22.2 ATOM 5115 CD1 TYR A 662 46.229 52.581 42.568 1.00 22.7 ATOM 5116 CD2 TYR A 662 46.229 52.581 42.568 1.00 22.7 ATOM 5117 CE1 TYR A 662 46.299 52.581 42.568 1.00 22.7 ATOM 5117 CE1 TYR A 662 46.299 52.581 42.568 1.00 22.7 ATOM 5118 CE2 TYR A 662 46.760 52.983 41.386 1.00 21.3 ATOM 5117 CE1 TYR A 662 46.898 52.771 39.048 1.00 22.2 ATOM 5120 OH TYR A 662 46.898 52.771 39.048 1.00 22.2 ATOM 5120 OH TYR A 662 46.898 52.771 39.048 1.00 22.2 ATOM 5120 OH TYR A 662 46.898 52.771 39.048 1.00 22.2 ATOM 5120 OH TYR A 663 42.922 53.492 42.736 1.00 22.3 ATOM 5121 N ASP A 663 42.922 53.492 42.736 1.00 22.3 ATOM 5122 CA ASP A 663 42.922 53.492 42.736 1.00 22.2 ATOM 5123 C ASP A 663 42.922 53.492 42.736 1.00 22.2 ATOM 5125 CB ASP A 663 42.922 53.492 42.736 1.00 22.3 ATOM 5126 CG ASP A 663 42.922 53.492 42.736 1.00 22.3 ATOM 5120 OH TYR A 662 46.898 52.771 39.048 1.00 22.2 ATOM 5121 N ASP A 663 42.922 53.492 42.736 1.00 22.3 ATOM 5125 CB ASP A 663 42.922 53.492 42.736 1.00 22.5 ATOM 5121 N ASP A 663 42.922 53.492 42.736 1.00 22.3 ATOM 5125 CB ASP A 663 42.925 53.492 42.736 1.00 22.3 ATOM 5126 CG ASP A 663 42.925 53.492 42.736 1.00 22.3 ATOM 5130 CA SER A 664 37.519 52.525 33.93 39.730 1.00 24.4 ATOM 5130 CA SER A 664 37.619 51.477 34.0397 1.00 23.7 ATOM 5130 CB SER A 664 37.655 58.394 41	1.13 1.47 1.26 1.70 1.068 1.57 1.52 1.32 1.32 1.32 1.32 1.32 1.32 1.32 1.3
ATOM 5104 CD2 TYR A 661 46.887 51.717 50.905 1.00 21.2 ATOM 5105 CE1 TYR A 661 45.166 52.840 52.6693 1.00 24.7 ATOM 5106 CE2 TYR A 661 47.100 51.566 52.259 1.00 20.6 ATOM 5107 CZ TYR A 661 46.248 52.117 53.144 1.00 22.0 ATOM 5108 OH TYR A 661 46.248 52.117 53.144 1.00 22.0 ATOM 5109 N TYR A 661 46.446 51.935 54.523 1.00 21.5 ATOM 5110 CA TYR A 662 43.906 52.192 46.063 1.00 21.5 ATOM 5111 C TYR A 662 42.828 53.020 43.979 1.00 22.3 ATOM 5112 O TYR A 662 41.761 53.079 44.599 1.00 22.2 ATOM 5113 CB TYR A 662 44.657 53.187 43.933 1.00 22.2 ATOM 5113 CB TYR A 662 44.657 51.187 43.933 1.00 22.2 ATOM 5115 CD1 TYR A 662 44.853 50.960 41.439 1.00 22.3 ATOM 5116 CD2 TYR A 662 44.853 50.960 41.439 1.00 22.3 ATOM 5117 CE1 TYR A 662 44.853 50.960 41.439 1.00 22.2 ATOM 5118 CE2 TYR A 662 44.853 50.960 41.439 1.00 21.3 ATOM 5119 CZ TYR A 662 46.760 52.983 41.386 1.00 21.3 ATOM 5119 CZ TYR A 662 46.370 52.345 40.214 1.00 23.5 ATOM 5120 OH TYR A 662 46.370 52.345 40.214 1.00 23.5 ATOM 5121 N ASP A 663 42.922 53.492 42.736 1.00 22.2 ATOM 5122 CA ASP A 663 42.922 53.492 42.736 1.00 22.2 ATOM 5123 C ASP A 663 42.922 53.492 42.736 1.00 22.2 ATOM 5123 C ASP A 663 42.922 53.492 42.736 1.00 22.2 ATOM 5123 C ASP A 663 42.922 53.492 42.736 1.00 22.2 ATOM 5124 O ASP A 663 42.922 53.492 42.736 1.00 22.2 ATOM 5125 CB ASP A 663 42.922 53.492 42.736 1.00 23.0 ATOM 5126 CG ASP A 663 42.922 53.492 42.736 1.00 23.0 ATOM 5127 OD1 ASP A 663 42.922 53.492 42.736 1.00 23.0 ATOM 5128 OD2 ASP A 663 42.939 54.223 39.732 1.00 24.8 ATOM 5130 CA SER A 664 38.199 53.343 41.864 1.00 23.5 ATOM 5131 C SER A 664 37.655 54.327 42.199 1.00 23.6 ATOM 5132 O SER A 664 37.655 54.324 41.743 1.00 23.6 ATOM 5133 C SER A 664 37.655 54.324 41.743 1.00 23.6 ATOM 5133 C SER A 664 37.655 54.324 41.743 1.00 23.6 ATOM 5133 CB SER A 664 37.655 54.334 41.744 1.00 23.6 ATOM 5133 C SER A 664 37.655 38.901 51.223 37.779 1.00 24.4 ATOM 5133 C BER A 665 38.901 51.223 37.779 1.00 24.4 ATOM 5134 OG SER A 6665 38.901 51.223 37.779 1.00 24.4 ATOM 5137 C VAL A 665 38.910 53.485 36.775 1	
ATOM	.70 .68 .51 .57 .52 .38 .23 .725 .30 .530 .234 .596 .04 .88 .15
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ATOM 5108 OH TYR A 661 43.906 52.192 46.063 1.00 21.5 ATOM 5110 CA TYR A 662 44.091 52.436 44.647 1.00 21.5 ATOM 5111 C TYR A 662 44.091 52.436 44.647 1.00 21.5 ATOM 5111 C TYR A 662 42.828 53.020 43.979 1.00 22.2 ATOM 5112 O TYR A 662 41.761 53.079 44.599 1.00 22.2 ATOM 5114 CG TYR A 662 41.761 53.079 44.599 1.00 22.0 ATOM 5114 CG TYR A 662 44.657 51.187 43.933 1.00 22.0 ATOM 5115 CD1 TYR A 662 45.273 51.547 42.627 1.00 21.8 ATOM 5116 CD2 TYR A 662 46.229 52.581 42.568 1.00 22.7 ATOM 5117 CE1 TYR A 662 44.853 50.960 41.439 1.00 21.2 ATOM 5118 CE2 TYR A 662 46.760 52.983 41.386 1.00 21.3 ATOM 5119 CZ TYR A 662 46.370 52.345 40.214 1.00 25.3 ATOM 5120 OH TYR A 662 46.898 52.771 39.048 1.00 22.2 ATOM 5121 N ASP A 663 42.922 53.459 40.214 1.00 23.5 ATOM 5122 CA ASP A 663 42.922 53.459 42.791 1.00 22.2 ATOM 5123 C ASP A 663 40.605 53.355 41.901 1.00 22.2 ATOM 5124 O ASP A 663 40.605 53.355 41.901 1.00 23.6 ATOM 5125 CB ASP A 663 40.619 52.120 41.715 1.00 23.0 ATOM 5126 CG ASP A 663 42.203 55.065 40.984 1.00 23.0 ATOM 5127 OD1 ASP A 663 42.203 55.065 40.984 1.00 23.0 ATOM 5128 OD2 ASP A 663 42.439 54.223 39.732 1.00 24.8 ATOM 5130 CA SER A 664 38.199 53.343 41.685 1.00 23.7 ATOM 5131 C SER A 664 38.199 53.343 41.685 1.00 23.6 ATOM 5132 O SER A 664 38.199 53.343 41.685 1.00 23.6 ATOM 5133 CB SER A 664 37.619 51.473 40.375 1.00 23.6 ATOM 5133 CB SER A 664 37.619 51.473 40.375 1.00 23.7 ATOM 5134 OG SER A 664 37.619 51.473 40.375 1.00 23.9 ATOM 5135 N VAL A 665 38.910 52.557 37.338 1.00 24.3 ATOM 5136 CA VAL A 665 38.910 52.557 37.338 1.00 24.3 ATOM 5137 C VAL A 665 38.910 52.557 37.338 1.00 24.2 ATOM 5138 O VAL A 665 38.343 50.255 37.338 1.00 24.2 ATOM 5140 CG1 VAL A 665 38.343 50.255 37.338 1.00 23.9 ATOM 5140 CG1 VAL A 665 38.343 50.255 37.338 1.00 23.9 ATOM 5140 CG1 VAL A 665 38.343 50.255 37.338 1.00 23.9 ATOM 5140 CG1 VAL A 665 38.343 50.255 37.338 1.00 23.7 ATOM 5140 CG1 VAL A 665 38.307 52.414 35.374 1.00 23.2	51 57 52 38 23 24 25 30 23 24 59 04 25 04 05 05 05 05 05 05 0
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ATOM 5113 CB TYR A 662 44.657 51.187 43.933 1.00 22.0 ATOM 5114 CG TYR A 662 45.273 51.547 42.627 1.00 21.8 ATOM 5115 CD1 TYR A 662 46.229 52.581 42.568 1.00 22.7 ATOM 5116 CD2 TYR A 662 44.853 50.960 41.439 1.00 21.2 ATOM 5117 CE1 TYR A 662 46.760 52.983 41.386 1.00 21.3 ATOM 5118 CE2 TYR A 662 45.427 51.326 40.236 1.00 25.3 ATOM 5119 CZ TYR A 662 46.370 52.345 40.214 1.00 23.5 ATOM 5120 OH TYR A 662 46.898 52.771 39.048 1.00 20.2 ATOM 5121 N ASP A 663 42.922 53.492 42.736 1.00 22.2 ATOM 5122 CA ASP A 663 42.922 53.492 42.736 1.00 22.5 ATOM 5123 C ASP A 663 40.605 53.355 41.901 1.00 23.6 ATOM 5124 O ASP A 663 40.605 53.355 41.901 1.00 23.6 ATOM 5125 CB ASP A 663 40.605 53.355 41.901 1.00 23.0 ATOM 5125 CB ASP A 663 42.203 55.065 40.984 1.00 23.0 ATOM 5125 CB ASP A 663 42.439 54.223 39.732 1.00 24.8 ATOM 5127 OD1 ASP A 663 42.439 54.223 39.732 1.00 24.8 ATOM 5128 OD2 ASP A 663 41.517 53.513 39.230 1.00 26.1 ATOM 5128 OD2 ASP A 663 41.517 53.513 39.230 1.00 24.8 ATOM 5131 C SER A 664 39.454 54.015 41.894 1.00 23.6 ATOM 5131 C SER A 664 39.454 54.015 41.894 1.00 23.6 ATOM 5131 C SER A 664 39.454 54.015 41.894 1.00 23.6 ATOM 5131 C SER A 664 38.080 52.588 40.375 1.00 24.3 ATOM 5133 CB SER A 664 37.065 54.334 41.743 1.00 24.4 ATOM 5133 CB SER A 664 37.065 54.334 41.743 1.00 24.4 ATOM 5134 OG SER A 664 37.065 54.334 41.743 1.00 24.4 ATOM 5135 N VAL A 665 38.176 52.557 37.959 1.00 24.4 ATOM 5136 CA VAL A 665 38.176 52.557 37.959 1.00 24.4 ATOM 5138 O VAL A 665 38.343 50.255 37.338 1.00 23.9 ATOM 5138 O VAL A 665 38.343 50.255 37.338 1.00 23.2 ATOM 5138 O VAL A 665 38.343 50.255 37.338 1.00 23.2 ATOM 5139 CB VAL A 665 38.343 50.255 37.338 1.00 23.2 ATOM 5134 CG1 VAL A 665 38.307 52.741 35.374 1.00 23.2 ATOM 5134 CG2 VAL A 665 38.307 52.741 35.374 1.00 24.4 ATOM 5134 CG1 VAL A 665 38.307 52.741 35.374 1.00 23.2 ATOM 5141 CG2 VAL A 665 38.307 52.741 35.374 1.00 23.2 ATOM 5141 CG2 VAL A 665 38.307 52.741 35.374 1.00 23.2 ATOM 5141 CG2 VAL A 665 38.307 52.741 35.374 1.00 23.2 ATOM 5141 CG2 VAL A 665 38.307 52.741 35.374 1	.04 .82 .72 .25 .34 .50 .23 .24 .59 .66 .04 .88
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20 ATOM 5116 CD2 TYR A 662 44.853 50.960 41.439 1.00 21.2 ATOM 5117 CE1 TYR A 662 46.760 52.983 41.386 1.00 21.3 ATOM 5118 CE2 TYR A 662 45.427 51.326 40.236 1.00 25.3 ATOM 5119 CZ TYR A 662 46.370 52.345 40.214 1.00 23.5 ATOM 5120 OH TYR A 662 46.898 52.771 39.048 1.00 20.2 ATOM 5121 N ASP A 663 42.922 53.492 42.736 1.00 22.2 ATOM 5122 CA ASP A 663 41.808 54.237 42.199 1.00 22.5 ATOM 5123 C ASP A 663 40.605 53.355 41.901 1.00 23.0 ATOM 5125 CB ASP A 663 40.605 53.355 41.901 1.00 23.0 ATOM 5125 CB ASP A 663 42.439 55.065 40.984 1.00 23.0 ATOM 5125 CB ASP A 663 42.439 52.120 41.715 1.00 23.0 ATOM 5126 CG ASP A 663 42.439 54.223 39.732 1.00 24.8 ATOM 5129 N SER A 664 34.517 53.513 39.230 1.00 26.1 ATOM 5129 N SER A 664 38.199 53.343 41.685 1.00 23.6 ATOM 5130 CA SER A 664 38.199 53.343 41.685 1.00 23.6 ATOM 5131 C SER A 664 38.199 53.343 41.685 1.00 23.6 ATOM 5131 C SER A 664 38.199 53.343 41.685 1.00 23.7 ATOM 5133 CB SER A 664 37.619 51.473 40.397 1.00 23.7 ATOM 5134 OG SER A 664 37.619 51.473 40.397 1.00 23.7 ATOM 5135 N VAL A 665 38.446 53.195 39.253 1.00 24.4 ATOM 5137 C VAL A 665 38.446 53.195 39.253 1.00 24.4 ATOM 5137 C VAL A 665 38.901 51.223 37.779 1.00 24.4 ATOM 5138 O VAL A 665 38.901 51.223 37.779 1.00 24.4 ATOM 5138 O VAL A 665 38.901 51.223 37.779 1.00 24.4 ATOM 5139 CB VAL A 665 38.901 51.223 37.779 1.00 24.4 ATOM 5139 CB VAL A 665 38.901 51.223 37.779 1.00 24.4 ATOM 5139 CB VAL A 665 38.901 51.223 37.779 1.00 24.4 ATOM 5139 CB VAL A 665 38.901 51.223 37.779 1.00 24.4 ATOM 5139 CB VAL A 665 38.901 51.223 37.779 1.00 24.4 ATOM 5139 CB VAL A 665 38.901 51.223 37.779 1.00 24.4 ATOM 5139 CB VAL A 665 38.901 51.223 37.779 1.00 24.4 ATOM 5139 CB VAL A 665 38.901 51.223 37.779 1.00 24.4 ATOM 5130 CB VAL A 665 38.901 51.223 37.779 1.00 24.4 ATOM 5140 CG1 VAL A 665 38.901 51.223 37.779 1.00 24.4 ATOM 5140 CG1 VAL A 665 38.901 51.223 37.779 1.00 24.4 ATOM 5141 CG2 VAL A 665 38.901 51.223 37.793 1.00 25.2 ATOM 5141 CG2 VAL A 665 38.901 51.223 37.933 1.00 25.2 ATOM 5141 CG2 VAL A 665 38.901 51.223 37.933 1.00	.25 .34 .30 .50 .23 .24 .59 .66 .04 .88
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35 ATOM 5131 C SER A 664 38.080 52.588 40.375 1.00 23.9 ATOM 5132 O SER A 664 37.619 51.473 40.397 1.00 23.7 ATOM 5133 CB SER A 664 37.065 54.334 41.743 1.00 24.4 ATOM 5134 OG SER A 664 37.255 55.329 40.782 1.00 24.3 ATOM 5135 N VAL A 665 38.446 53.195 39.253 1.00 23.9 40 ATOM 5136 CA VAL A 665 38.176 52.557 37.959 1.00 24.4 ATOM 5137 C VAL A 665 38.901 51.223 37.779 1.00 24.1 ATOM 5138 O VAL A 665 38.343 50.255 37.338 1.00 25.0 ATOM 5139 CB VAL A 665 38.343 50.255 37.338 1.00 25.2 ATOM 5140 CG1 VAL A 665 38.307 52.741 35.374 1.00 23.2 45 ATOM 5141 CG2 VAL A 665 37.629 54.748 36.854 1.00 26.3 ATOM 5142 N TYR A 666 40.155 51.172 38.130 1.00 23.7 ATOM 5143 CA TYR A 666 40.910 49.952 37.933 1.00 24.2	.69
ATOM 5132 O SER A 664 37.619 51.473 40.397 1.00 23.7 ATOM 5133 CB SER A 664 37.065 54.334 41.743 1.00 24.4 ATOM 5134 OG SER A 664 37.255 55.329 40.782 1.00 24.3 ATOM 5135 N VAL A 665 38.446 53.195 39.253 1.00 23.9 40 ATOM 5136 CA VAL A 665 38.176 52.557 37.959 1.00 24.4 ATOM 5137 C VAL A 665 38.901 51.223 37.779 1.00 24.1 ATOM 5138 O VAL A 665 38.343 50.255 37.338 1.00 25.0 ATOM 5139 CB VAL A 665 38.343 50.255 37.338 1.00 25.0 ATOM 5140 CG1 VAL A 665 38.310 53.485 36.775 1.00 25.2 ATOM 5141 CG2 VAL A 665 38.307 52.741 35.374 1.00 23.2 45 ATOM 5142 N TYR A 666 40.155 51.172 38.130 1.00 23.7 ATOM 5143 CA TYR A 666 40.910 49.952 37.933 1.00 24.2	
ATOM 5134 OG SER A 664 37.255 55.329 40.782 1.00 24.3 ATOM 5135 N VAL A 665 38.446 53.195 39.253 1.00 23.9 40 ATOM 5136 CA VAL A 665 38.176 52.557 37.959 1.00 24.4 ATOM 5137 C VAL A 665 38.901 51.223 37.779 1.00 24.1 ATOM 5138 O VAL A 665 38.343 50.255 37.338 1.00 25.0 ATOM 5139 CB VAL A 665 38.510 53.485 36.775 1.00 25.2 ATOM 5140 CG1 VAL A 665 38.307 52.741 35.374 1.00 23.2 45 ATOM 5141 CG2 VAL A 665 37.629 54.748 36.854 1.00 26.3 ATOM 5142 N TYR A 666 40.155 51.172 38.130 1.00 23.7 ATOM 5143 CA TYR A 666 40.910 49.952 37.933 1.00 24.2	.78
40 ATOM 5136 CA VAL A 665 38.176 52.557 37.959 1.00 24.4 ATOM 5137 C VAL A 665 38.901 51.223 37.779 1.00 24.1 ATOM 5138 O VAL A 665 38.343 50.255 37.338 1.00 25.0 ATOM 5139 CB VAL A 665 38.510 53.485 36.775 1.00 25.2 ATOM 5140 CG1 VAL A 665 38.307 52.741 35.374 1.00 23.2 ATOM 5141 CG2 VAL A 665 37.629 54.748 36.854 1.00 26.3 ATOM 5142 N TYR A 666 40.155 51.172 38.130 1.00 23.7 ATOM 5143 CA TYR A 666 40.910 49.952 37.933 1.00 24.2	
ATOM 5137 C VAL A 665 38.901 51.223 37.779 1.00 24.1 ATOM 5138 O VAL A 665 38.343 50.255 37.338 1.00 25.0 ATOM 5139 CB VAL A 665 38.510 53.485 36.775 1.00 25.2 ATOM 5140 CG1 VAL A 665 38.307 52.741 35.374 1.00 23.2 ATOM 5141 CG2 VAL A 665 37.629 54.748 36.854 1.00 26.3 ATOM 5142 N TYR A 666 40.155 51.172 38.130 1.00 23.7 ATOM 5143 CA TYR A 666 40.910 49.952 37.933 1.00 24.2	
ATOM 5139 CB VAL A 665 38.510 53.485 36.775 1.00 25.2 ATOM 5140 CG1 VAL A 665 38.307 52.741 35.374 1.00 23.2 ATOM 5141 CG2 VAL A 665 37.629 54.748 36.854 1.00 26.3 ATOM 5142 N TYR A 666 40.155 51.172 38.130 1.00 23.7 ATOM 5143 CA TYR A 666 40.910 49.952 37.933 1.00 24.2	.19
ATOM 5140 CG1 VAL A 665 38.307 52.741 35.374 1.00 23.2 45 ATOM 5141 CG2 VAL A 665 37.629 54.748 36.854 1.00 26.3 ATOM 5142 N TYR A 666 40.155 51.172 38.130 1.00 23.7 ATOM 5143 CA TYR A 666 40.910 49.952 37.933 1.00 24.2	
ATOM 5142 N TYR A 666 40.155 51.172 38.130 1.00 23.7 ATOM 5143 CA TYR A 666 40.910 49.952 37.933 1.00 24.2	.28
ATOM 5144 C TYR A 666 40.585 48.956 38.982 1.00 23.8	
ATOM 5145 O TYR A 666 40.384 47.791 38.677 1.00 22.2	.28
50 ATOM 5146 CB TYR A 666 42.382 50.267 38.030 1.00 24.4 ATOM 5147 CG TYR A 666 43.301 49.105 37.900 1.00 25.3	
ATOM 5148 CD1 TYR A 666 43.624 48.336 38.997 1.00 27.8	.84
ATOM 5149 CD2 TYR A 666 43.861 48.776 36.670 1.00 25.6 ATOM 5150 CE1 TYR A 666 44.493 47.296 38.891 1.00 26.7	
55 ATOM 5151 CE2 TYR A 666 44.715 47.730 36.545 1.00 25.3° ATOM 5152 CZ TYR A 666 45.055 47.009 37.667 1.00 25.4°	
ATOM 5153 OH TYR A 666 45.894 45.942 37.574 1.00 24.4	.41
ATOM 5154 N THR A 667 40.531 49.419 40.234 1.00 24.00 ATOM 5155 CA THR A 667 40.355 48.504 41.354 1.00 24.40	
60 ATOM 5156 C THR A 667 38.998 47.836 41.314 1.00 25.2	.21
ATOM 5157 O THR A 667 38.896 46.605 41.452 1.00 26.15 ATOM 5158 CB THR A 667 40.529 49.220 42.736 1.00 24.65	
ATOM 5159 OG1 THR A 667 41.790 49.890 42.820 1.00 24.00 ATOM 5160 CG2 THR A 667 40.590 48.214 43.886 1.00 24.90	
65 ATOM 5161 N GLU A 668 37.949 48.627 41.147 1.00 25.29	. 25
ATOM 5162 CA GLU A 668 36.603 48.073 41.246 1.00 25.9° ATOM 5163 C GLU A 668 36.276 47.103 40.084 1.00 26.8°	
ATOM 5164 O GLU A 668 35.475 46.201 40.206 1.00 26.00	.02
ATOM 5165 CB GLU A 668 35.569 49.207 41.358 1.00 26.00 70 ATOM 5166 CG GLU A 668 35.673 49.996 42.671 1.00 25.70	. UU

5	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5169 5169 5170	B OE 9 OE 0 N L CA 2 C	1 GLU 2 GLU ARG ARG ARG		34.9 34.0 35.2 36.9 36.8 37.0 36.3	45 51.44 67 52.20 64 47.27 02 46.36 70 44.94	3 41.722 8 43.394 1 38.974 6 37.844 5 38.254	1.00 1.00 1.00 1.00 1.00	25.22 28.90 30.04 29.89
10	ATOM ATOM	5174 5175 5176 5177 5178	CB CG CD NE CZ	ARG ARG ARG ARG ARG	A 669 A 669 A 669 A 669 A 669	37.8 37.2 37.2 37.9 39.38	53 46.695 85 46.953 98 46.346 80 46.723	36.804 35.499 34.354 34.302	1.00 1.00 1.00	
15	ATOM ATOM	5179 5180 5181 5182 5183	NH: N CA C	1 ARG 2 ARG TYR TYR TYR	A 669 A 669 A 670 A 670 A 670	39.09 41.15 38.20 38.61 38.15	55 48.979 58 48.098 01 44.770 10 43.454	33.944 34.108 38.934 39.384	1.00 1.00 1.00	38.09 35.77 29.76 30.01 30.26
20	ATOM ATOM ATOM ATOM ATOM	5184 5185 5186 5187 ; 5188	CB CG CD1	TYR TYR L TYR	A 670 A 670 A 670 A 670 A 670	38.17 40.13 40.66 40.38 41.39	32 43.310 34 43.860 34 43.242	41.132 39.314 38.056 36.826	1.00 1.00 1.00	31.10 29.59 28.51 30.93
25	ATOM ATOM ATOM ATOM	5189 5190 5191 5192	CE1 CE2 CZ OH	TYR A TYR A TYR A TYR A	A 670 A 670 A 670 A 670	40.85 41.86 41.61 42.03	6 43.778 6 45.567 5 44.927 8 45.491	35.628 36.899 35.704 34.588	1.00 1.00 1.00	29.14 28.01 27.43 26.81 30.30
30	ATOM ATOM ATOM ATOM ATOM ATOM	5193 5194 5195 5196 5197 5198	N CA C O CB CG	MET A	4 671	37.80 37.51 36.10 35.79 38.54 39.88	7 43.742 0 44.043 6 43.702 8 44.379	42.969 43.486	1.00 1.00 1.00 1.00	31.12 31.05 31.36 30.25 30.81
35	ATOM ATOM ATOM ATOM ATOM	5199 5200 5201 5202	SD CE N CA	MET A MET A GLY A	671 671 672 672	39.93 39.98 35.23 33.92	3 42.170 8 42.879 6 44.629 2 45.029	44.727 46.392 42.654 43.126	1.00 1.00 1.00	30.32 30.89 28.68 31.62 32.28
40	ATOM ATOM ATOM ATOM ATOM	5203 5204 5205 5206 5207 5208	C O N CA C	GLY A GLY A LEU A LEU A LEU A	672 673 673 673	34.06 35.07 33.07 33.17 33.61 33.27	4 46.868 5 46.383 5 47.451 2 46.919	44.121 44.117 44.970 45.946 47.304 47.667	1.00 1.00 1.00 1.00	33.48 34.40 33.67 33.93 33.21 32.81
45	ATOM ATOM ATOM ATOM ATOM	5209 5210 5211 5212 5213	CB CG CD1 CD2 N	LEU A	673 673 673 673	31.83 31.34 29.90 32.20 34.34	5 48.152 1 49.002 3 49.435 5 50.208	46.103 44.958 45.261 44.786 48.065	1.00 1.00 1.00 1.00	34.34 35.92 38.82 36.78 32.97
50	ATOM ATOM ATOM ATOM ATOM	5214 5215 5216 5217 5218	CA C O CB CG	PRO A PRO A PRO A PRO A	674 674 674 674	34.777 33.721 33.996 36.009 35.621	47.323 47.625 48.429 48.189	49.399 50.497 51.402 49.613	1.00 1.00 1.00 1.00	33.06 33.83 32.53 32.38
55	ATOM ATOM ATOM ATOM ATOM	5219 5220 5221 5222 5223	CD N CA C	PRO A THR A THR A THR A THR A	674 675 675 675	34.826 32.550 31.519 31.185 31.431	49.083 46.997 47.046 45.643	49.044 47.758 50.395 51.443 51.936 51.258	1.00 1.00 1.00 1.00 1.00	33.10 34.72 36.32 36.59
60	ATOM ATOM ATOM ATOM ATOM	5224 5225 5226 5227 5228	CG2 N	THR A THR A THR A PRO A PRO A	675 675 675 676	30.208 29.806 30.385 30.584 30.165	47.605 46.817 49.028 45.552	50.910 49.771 50.381 53.112	1.00 1.00 1.00	36.75 38.87 36.51 37.32
65	ATOM ATOM ATOM ATOM ATOM	5229 5230 5231 5232 5233	C O CB CG	PRO A PRO A PRO A PRO A PRO A	676 676 676 676	29.234 29.293 29.451 30.102 30.301		53.656 52.740 52.743 54.952 55.347	1.00 : 1.00 : 1.00 : 1.00 :	37.37 38.17 38.18
70	ATOM ATOM ATOM	5234 5235 5236	N CA	GLU A GLU A GLU A	677 677	28.429 27.490 28.139	44.144 43.463 42.998	54.053 51.939 51.060 49.751	1.00 3 1.00 3 1.00 4 1.00 3	10.38

	ATOM	5237	0	GLU	Δ 6	77	27.626	42.096	49.104	1 00	39.65
	ATOM	5238	СВ	GLU			26.261	44.358	50.807		41.65
	ATOM	5239	CG	GLU			26.229	45.053	49.454		45.83
	ATOM	5240	CD	GLU	A 6	577	25.316	46.285	49.437		52.13
5	ATOM	5241	OE1	GLU	A 6	77	25.569	47.207	50.256	1.00	55.30
	ATOM	5242	OE2	GLU	A 6	77	24.365	46.341	48.596	1.00	53.85
	ATOM	5243	N	ASP			29.275	43.591	49.366		38.46
	ATOM	5244	CA	ASP			29.949	43.202	48.124		36.21
	ATOM	5245	С	ASP	A 6	78	31.289	42.493	48.385	1.00	35.24
10	ATOM	5246	0	ASP	A 6	78	31.277	41.314	48.622	1.00	34.64
	ATOM	5247	СВ	ASP			30.068	44.384	47.168		36.35
				ASP		-	30.594	43.979	45.787		37.08
	ATOM	5248	CG								
	ATOM	5249	OD1	ASP	A 6	78	30.891	42.770	45.598		36.62
	ATOM	5250	OD2	ASP	A 6	78	30.739	44.794	44.834	1.00	36.77
15	ATOM	5251	N	ASN	A 6	79	32.445	43.156	48.378	1.00	33.79
	ATOM	5252	CA	ASN			33.701	42.366	48.454		32.51
	ATOM	5253	C	ASN			34.670	42.785	49.562		31.96
	ATOM	5254	0	ASN			35.856	42.512	49.463		29.64
	ATOM	5255	CB	ASN	А6	79	34.399	42.395	47.080	1.00	32.28
20	ATOM	5256	CG	ASN	A 6	79	35.400	41.251	46.849	1.00	29.98
	ATOM	5257	OD1				36.394	41.448	46.157		34.09
	ATOM	5258	ND2				35.141	40.077	47.383		26.34
	ATOM	5259	N	LEU	A 6	80	34.163	43.385	50.649	1.00	32.19
	ATOM	5260	CA	LEU	A 6	80	35.048	43.880	51.735	1.00	33.13
25	ATOM	5261	С	LEU	A 6	80	36.015	42.836	52.286	1.00	32.66
	ATOM	5262	ŏ	LEU			37.218	43.120	52.454		32.25
	MOTA	5263	CB	LEU			34.253	44.508	52.882		33.62
	ATOM	5264	CG	LEU	A 6	80	35.024	45.198	54.019	1.00	36.92
	ATOM	5265	CD1	LEU .	A 6	80	35.911	46.349	53.515	1.00	37.94
30	ATOM	5266	CD2	LEU .	A 6	80	34.020	45.718	55.110	1.00	36.39
	ATOM	5267	N	ASP			35.513	41.633	52.553		31.71
	_										
	ATOM	5268	CA	ASP .			36.356	40.598	53.099		32.46
	ATOM	5269	С	ASP .	A 6	81	37.599	40.402	52.251		31.68
	ATOM	5270	0	ASP .	A 6	81	38.688	40.384	52.786	1.00	31.47
35	MOTA	5271	СВ	ASP .	A 6	81	35.631	39.250	53.241		33.28
-	ATOM	5272	CG	ASP .			34.621	39.226	54.411		36.99
	MOTA	5273		ASP .			34.514	40.224	55.155		37.92
	ATOM	5274	OD2	ASP .	A 6	81	33.899	38.220	54.659	1.00	41.78
	ATOM	5275	N	HIS .	A 6	82	37.461	40.231	50.945	1.00	30.30
40	ATOM	5276	CA	HIS .	A 6	82	38.663	40.020	50.182	1.00	30.43
	ATOM	5277	C	HIS			39.565	41.263	50.055		28.84
	ATOM	5278	0	HIS .			40.752	41.128	49.917		28.95
	MOTA	5279	CB	HIS A		82	38.419	39.434	48.816		30.48
	ATOM	5280	CG	HIS .	A 6	82	39.704	39.091	48.132	1.00	33.22
45	ATOM	5281	ND1	HIS A	A 6	82	40.619	38.219	48.684		35.26
	ATOM	5282		HIS			40.277	39.570	47.004		30.92
	MOTA	5283		HIS A			41.672	38.128	47.897		31.98
	ATOM	5284	NE2	HIS A	A 6	82	41.496	38.950	46.880	1.00	32.30
	ATOM	5285	N	TYR Z	A 6	83	39.012	42.456	50.053	1.00	27.68
50	ATOM	5286	CA	TYR Z			39.834	43.649	50.072		27.60
	ATOM	5287	C	TYR			40.704	43.634	51.355		27.75
	MOTA	5288	0	TYR A			41.834	44.118	51.367		25.84
	ATOM	5289	CB	TYR A	A 6	83	38.963	44.884	50.146	1.00	26.87
	ATOM	5290	CG	TYR Z	A 6	83	38.554	45.591	48.850	1.00	29.98
55	ATOM	5291	CD1				37.402	45.230	48.157		29.80
55	ATOM	5292		TYR Z			39.283	46.691	48.382		27.64
	MOTA	5293	CE1				37.000	45.939	47.005		29.62
	ATOM	5294	CE2	TYR A	4 6	83	38.900	47.373	47.278	1.00	29.75
	MOTA	5295	CZ	TYR A	A 6	83	37.744	47.000	46.587	1.00	29.38
60	ATOM	5296	ОН	TYR A			37.389	47.704	45.476		29.36
55											
	MOTA	5297	N	ARG A			40.179	43.056	52.433		28.35
	MOTA	5298	CA	ARG A	A 6	84	40.851	43.174	53.724		29.33
	MOTA	5299	С	ARG A	A 6	84	41.889	42.102	53.953	1.00	29.28
	ATOM	5300	Ō	ARG A			42.902	42.380	54.574		27.35
65	ATOM	5301	ČВ	ARG A			39.836	43.261	54.878		30.81
55											
	ATOM	5302	CG	ARG A			39.623	44.659	55.354		33.87
	MOTA	5303	CD	ARG A			38.403	45.271	54.873	1.00	40.64
	ATOM	5304	NE	ARG A	A 6	84	38.428	46.748	54.722	1.00	45.03
	ATOM	5305	CZ	ARG A			38.149	47.623	55.676		44.59
70	ATOM	5306		ARG A			37.901	47.192	56.899		43.82
, 0	A LON	2200	TATIT	DUG 1	z 0	- 	J1.JUI	31.17 <i>C</i>	JU.077	1.00	47.02

	ATOM	5307		2 ARG			38.11	2 48.9	27	55.393	1.00 44.58
	ATOM	5308				685	41.70			53.305	
	ATOM ATOM	5309 5310				685	42.583 43.697			53.409	
5		5311				685	44.542			52.302 52.255	
	ATOM	5312				685	41.724			53.340	1.00 27.83
	ATOM	5313				685	42.546	37.1	97	53.590	
	ATOM	5314				685	43.730			53.925	1.00 45.27
10	MOTA MOTA	5315 5316				685	41.915			53.407	
10	ATOM	5317				686 686	43.723 44.703			51.456 50.362	
	ATOM	5318				686	45.704			50.362	1.00 25.93 1.00 25.52
	MOTA	5319	0	SEF	A	686	46.200			49.442	1.00 25.32
,,	MOTA	5320	CB			686	43.988	40.8		49.007	1.00 24.81
15	ATOM	5321	OG			686	43.164			48.829	1.00 23.66
	ATOM ATOM	5322 5323	N CA			687 687	45.990			51.657	1.00 25.47
	ATOM	5324	C			687	46.950 48.323			51.883 52.129	1.00 25.57 1.00 24.54
	ATOM	5325	ŏ			687	48.480	41.8		52.564	1.00 24.54
20	ATOM	5326	CB			687	46.613	44.3		53.133	1.00 25.76
	ATOM	5327	OG1			687	46.899			54.242	1.00 26.17
	ATOM ATOM	5328 5329	CG2 N			687 688	45.126			53.256	1.00 26.56
	ATOM	5330	CA			688	49.326 50.688			51.816 52.102	1.00 25.38
25	ATOM	5331	C			688	50.865			53.615	1.00 25.28 1.00 24.05
	ATOM	5332	0	VAL	Α	688	51.516			54.224	1.00 22.44
	ATOM	5333	CB			688	51.666	44.2	69 5	51.410	1.00 24.90
	ATOM ATOM	5334 5335	CG1	VAL	A	688	53.097			51.842	1.00 27.31
30	ATOM	5336	N .	VAL MET		689	51.516 50.222	44.1 44.3		49.937 54.229	1.00 23.55
	ATOM	5337	CA			689	50.450	44.6		55.655	1.00 24.40 1.00 25.35
	MOTA	5338	С			689	50.133	43.3		56.484	1.00 25.35
	ATOM	5339	0			689	50.857	43.0	71 5	57.409	1.00 26.90
- 35	ATOM ATOM	5340	CB	MET			49.669	45.80		6.167	1.00 25.18
33	ATOM	5341 5342	CG SD	MET MET			50.343 50.258	47.15 47.5		55.795	1.00 25.17
	ATOM	5343	CE	MET			48.576	48.03		53.985 53.891	1.00 26.00 1.00 25.22
	ATOM	5344	N			690	49.120	42.5		6.120	1.00 23.22
	ATOM	5345	CA			690	48.743	41.47		6.984	1.00 28.78
40	ATOM	5346	C	SER			49.790	40.35		7.003	1.00 28.89
	ATOM ATOM	5347 5348	O CB	SER SER			49.779	39.48		7.886	1.00 29.60
	ATOM	5349	OG	SER			47.353 47.324	40.92		6.599 5.227	1.00 28.81 1.00 31.54
	ATOM	5350	Ŋ	ARG			50.703	40.38	31 5	6.044	1.00 31.54
45	MOTA	5351	CA	ARG			51.711	39.37		5.986	1.00 27.51
	ATOM	5352	C	ARG			53.045	39.80		6.611	1.00 27.64
	ATOM ATOM	5353 5354	O CB	ARG ARG			54.049	39.09		6.442	1.00 27.10
	ATOM	5355	CG	ARG			51.876 50.571	38.94		4.528	1.00 27.22 1.00 26.70
50	ATOM	5356	CD	ARG			50.652	38.02		2.482	1.00 26.70
	ATOM	5357	NE	ARG			49.423	37.46		1.911	1.00 31.01
	ATOM	5358	CZ	ARG			49.439	36.63	5 5	0.876	1.00 31.66
	ATOM ATOM	5359	NH1	ARG			50.605	36.30		0.332	1.00 28.29
55	ATOM	5360 5361	NHZ N	ARG ALA			48.309 53.046	36.11		0.400	1.00 32.39
33	ATOM	5362	CA	ALA			54.290	40.92		7.328 7.849	1.00 27.06 1.00 29.54
	ATOM	5363	C	ALA			55.258	40.55		8.496	1.00 29.91
	MOTA	5364	0	ALA			56.439	40.58	0 5	8.189	1.00 29.93
60	ATOM	5365	CB	ALA			53.987	42.62	5 5	8.856	1.00 30.04
60	ATOM	5366 5367	N	GLU			54.748	39.74	8 5	9.420	1.00 31.37
	ATOM ATOM	5367 5368	CA C	GLU			55.545	38.81	_	0.203	1.00 32.71
	ATOM	5369	0	GLU GLU			56.389 57.492	37.91 37.54		9.353	1.00 32.63
	ATOM	5370	СВ	GLU			54.639	37.89		9.748 1.025	1.00 31.76 1.00 33.70
65	ATOM	5371	CG	GLU			53.837	38.57		2.118	1.00 33.70
	ATOM	5372	CD	GLU	A	693	54.597	38.70	1 6	3.439	1.00 44.49
	ATOM	5373		GLU			55.795	38.29		3.502	1.00 42.20
	ATOM ATOM	5374 5375	OE2 N	GLU ASN			53.968	39.21		4.412	1.00 46.31
70	ATOM	5376	CA	ASN			55.836 56.511	37.51 36.60		8.210	1.00 32.72
. •		5575	Ų.1	- 7774	(J - 2	JU. JII	20.00	0 5	7.307	1.00 33.40

	ATOM	5377	С	ASN A	694	57.767	37.238	56.690	1.00	33.58
	ATOM	5378	0	ASN A	694	58.667	36.534	56.298	1.00	34.60
	ATOM	5379	CB	ASN A		55.521	36.125	56.211	1.00	33.62
_	ATOM	5380	CG	ASN A		54.414	35.164	56.759		35.53
5	MOTA	5381		ASN A		54.608	34.474	57.741		40.35
	MOTA	5382		ASN A		53.290	35.094	56.071		40.72
	ATOM	5383	N	PHE A		57.859	38.564	56.617	1.00	
	ATOM	5384	CA	PHE A		59.011	39.160	55.992	1.00	32.04
10	ATOM	5385	C	PHE A		60.322	38.897	56.779		32.80
10	MOTA	5386	O	PHE A		61.408 58.794	39.201	56.341 55.773		31.80 31.84
	ATOM ATOM	5387 5388	CB CG	PHE A		57.918	40.658 40.999	54.580		30.01
	ATOM	5389		PHE A		56.550	40.781	54.580		28.42
	ATOM	5390		PHE A		58.471	41.591	53.464		32.11
15	ATOM	5391		PHE A		55.755	41.092	53.564	1.00	27.96
13	ATOM	5392	CE2			57.691	41.914	52.373	1.00	
	ATOM	5393	CZ	PHE A		56.320	41.688	52.424		30.28
	ATOM	5394	N	LYS A		60.233	38.283	57.933		34.34
	ATOM	5395	CA	LYS A		61.440	38.049	58.709		35.39
20	ATOM	5396	C	LYS A		62.275	36.945	58.093		35.11
	ATOM	5397	ŏ	LYS A		63.409	36.718	58.478		35.26
	ATOM	5398	СB	LYS A		61.053	37.670	60.127		36.41
	ATOM	5399	CG	LYS A	696	60.241	36.403	60.206	1.00	39.12
	ATOM	5400	CD	LYS A	696	59.597	36.216	61.622	1.00	44.25
25	ATOM	5401	CE	LYS A	696	58.616	35.023	61.628	1.00	45.71
	ATOM	5402	NZ	LYS A	696	57.871	34.854	62.947	1.00	47.23
	MOTA	5403	N	GLN A	697	61.708	36.254	57.125		34.71
	ATOM	5404	CA	GLN A		62.380	35.138	56.499		35.52
	ATOM	5405	С	GLN A		63.187	35.522	55.295		34.21
30	ATOM	5406	0	GLN A		63.848	34.677	54.731		35.13
	ATOM	5407	СВ	GLN A		61.331	34.121	56.029		36.66
	ATOM	5408	CG	GLN A		60.840	33.188	57.117		40.42
	ATOM	5409	CD	GLN A		59.659	32.367	56.642		44.24
25	ATOM	5410		GLN A		59.817	31.445	55.803		48.10
35	ATOM	5411	NE2			58.483	32.693	57.148		41.55
	ATOM	5412	N	VAL A		63.112	36.782	54.894		32.68
	ATOM	5413 5414	CA	VAL A		63.728 64.325	37.230 38.649	53.655 53.776		31.46 30.29
	ATOM ATOM	5415	C	VAL A		64.119	39.323	54.753		29.83
40	ATOM	5416	O CB	VAL A		62.672	37.317	52.570		31.46
40	ATOM	5417		VAL A		61.821	36.048	52.487	1.00	
	ATOM	5418		VAL A		61.765	38.557	52.831		30.70
	ATOM	5419	N	GLU A		65.062	39.057	52.767		28.97
	ATOM	5420	CA	GLU A		65.604	40.415	52.648	1.00	
45	ATOM	5421	C	GLU A		64.813	41.169	51.591		27.24
	ATOM	5422	ō	GLU A		64.712	40.710	50.445		27.18
	ATOM	5423	ČВ	GLU A		67.052	40.349	52.234		29.36
	ATOM	5424	CG	GLU A		67.823	39.373	53.122	1.00	33.38
	ATOM	5425	CD	GLU A		69.169	39.010	52.541	1.00	40.83
50	ATOM	5426	OE1	GLU A	699	69.909	39.934	52.077	1.00	42.56
	MOTA	5427	OE2	GLU A	699	69.462	37.785	52.524		46.50
	MOTA	5428	N	TYR A		64.288	42.321	51.965		25.29
	ATOM	5429	CA	TYR A	700	63.348	43.087	51.117		24.48
	ATOM	5430	С	TYR A		63.823	44.489	50.917		23.48
55	MOTA	5431	0	TYR A		64.304	45.101	51.843		21.89
	ATOM	5432	CB	TYR A		62.045	43.186	51.903	1.00	24.85
	MOTA	5433	CG	TYR A		60.811	43.889	51.344	1.00	24.00
	MOTA	5434	CD1	TYR A	700	60.348	43.655	50.069		24.47
	ATOM	5435	CD2	TYR A		60.002	44.629	52.201		24.32
60	MOTA	5436	CE1	TYR A	700	59.153	44.248	49.606		25.02
	MOTA	5437	CE2	TYR A	700	58.818	45.204	51.767		26.02
	MOTA	5438	CZ	TYR A		58.383	45.004	50.467		25.69
	ATOM	5439	ОН	TYR A		57.190	45.585	50.088	1.00	22.93
- -	ATOM	5440	N	LEU A		63.647	45.017	49.725		22.74
65	MOTA	5441	CA	LEU A	701	63.969	46.408	49.458		22.82
	ATOM	5442	C	LEU A		62.708	47.006	48.890		23.35
	MOTA	5443	O	LEU A	701	62.166	46.520	47.892		23.55
	ATOM	5444	CB	LEU A		65.118 65.497	46.490	48.462 47.856		22.91
70	ATOM	5445 5446	CG CD1	LEU A		65.497 65.913	47.829	48.907		22.89
70	MOTA	5446	CDI	LEU A	, OT	65.913	48.884	40.30/	1.00	24.19

5	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	5449 5449 5450 5450	8 N 9 CA 0 C 1 O 2 CB	LEU LEU LEU LEU	A 701 A 702 A 702 A 702 A 702 A 702 A 702 A 702		66.608 62.253 61.010 61.393 62.173 60.135	1 48.073 0 48.759 2 50.145 1 50.862 5 48.847	49.531 49.184 48.715 49.382 50.464	1.00 1.00 1.00 1.00 1.00	22.51 21.85 19.94 23.03
10	ATOM ATOM	5454 5455 5456 5457	CD1 CD2 N CA	LEU LEU ILE ILE	A 702 A 702 A 703 A 703 A 703		57.813 58.164 60.866 61.237 59.977	3 48.855 49.820 5 50.535 7 51.802	49.423 51.680 47.561 46.963	1.00 1.00 1.00	21.66 21.68 22.17 20.85 20.96 21.27
15	ATOM ATOM	5459 5460 5461 5462 5463	CB CG1 CG2 CD1	ILE . ILE . ILE . ILE .	A 703 A 703 A 703 A 703 A 703		59.062 62.205 63.374 62.658 64.345	51.822 51.531 50.669 52.797 50.290	45.904 45.764 46.183 45.136	1.00 1.00 1.00	
20	ATOM ATOM ATOM ATOM ATOM	5464 5465 5466 5467 5468	CA C O	HIS A	A 704 A 704 A 704 A 704 A 704		59.918 58.737 59.070 59.865 57.620	54.539 56.017 56.581	46.592 46.133 45.954 46.696 47.174	1.00 1.00 1.00	20.79 21.54 21.73 22.47 21.36
25	ATOM ATOM ATOM ATOM ATOM	5469 5470 5471 5472 5473	CG 1 ND1 1 CD2 1	HIS A HIS A HIS A	A 704 A 704 A 704 A 704		56.234 55.313 55.586 54.184	54.364 53.380 55.271 53.649	46.613 46.901 45.843 46.274	1.00 1.00 1.00	22.52 20.34 22.80 22.86
30 ⁻	ATOM ATOM ATOM ATOM ATOM	5474 5475 5476 5477 5478	N (CA (CO) (CO) (CO) (CO) (CO) (CO) (CO) (CO)	GLY A GLY A GLY A	A 705 A 705 A 705 A 705		54.313 58.486 58.654 57.634 56.461	56.652 58.077 58.815 58.390	45.655 44.950 44.775 45.596 45.698	1.00 1.00 1.00	20.42 22.31 21.36 21.59 21.44
35	MOTA MOTA MOTA	5479 5480 5481 5482	CA 1 C 1 CB 1	THR A	706 706 706 706 706		58.032 57.175 56.129 55.177 57.985	59.957 60.666 61.449 61.844 61.602	46.133 47.055 46.345 46.967 47.999	1.00 1.00 1.00	21.99 22.11 22.60 23.64 22.70
40	ATOM ATOM ATOM ATOM ATOM	5483 5484 5485 5486 5487	CG2 T N A CA A C A	HR A LA A LA A LA A	706 706 707 707		58.616 59.134 56.313 55.277 54.522	62.657 60.832 61.730 62.453 61.557	47.267 48.685 45.071 44.344 43.388	1.00 1.00 1.00 1.00	21.83 22.51 22.16 23.18 22.84
45	ATOM ATOM ATOM ATOM ATOM ATOM	5488 5489 5490 5491 5492 5493	CB A N A CA A C A	LA A SP A SP A SP A	707 707 708 708 708 708		54.086 55.868 54.366 53.624 52.100	62.027 63.635 60.285 59.337 59.638	42.317 43.565 43.758 42.932 43.031	1.00 1.00 1.00 1.00	22.90 23.66 22.28 23.26 23.76
50	ATOM ATOM ATOM ATOM ATOM	5494 5495 5496 5497 5498	CB A CG A OD1 A OD2 A	SP A SP A SP A SP A	708 708 708 708	, ,	51.484 54.005 53.609 52.633 54.176	59.426 57.959 56.843 57.029 55.707	44.041 43.391 42.417 41.678 42.429	1.00 1.00 1.00 1.00	22.55 22.95 23.76 22.38 18.33
55	ATOM ATOM ATOM ATOM ATOM	5499 5500 5501 5502 5503	CA A C A C A CB A	SP A SP A SP A SP A SP A	709 709 709 709	<u>.</u> 4	51.510 50.113 19.204 18.003 19.914	60.161 60.572 59.426 59.573 61.650	41.953 41.942 41.547 41.549 40.890	1.00 1.00 1.00 1.00	24.61 24.71 24.28 24.39 25.52
60	ATOM ATOM ATOM ATOM ATOM	5504 5505 5506 5507 5508	OD1 AS OD2 AS N AS CA AS	SP A SP A SN A SN A	709 709 710 710	5 4 4 4	50.408 51.643 19.653 19.771 19.010	61.179 61.032 60.840 58.255 57.125	39.528 39.357 38.616 41.338 40.826		25.08 25.79 24.32 24.34
65	ATOM ATOM ATOM ATOM	5509 5510 5511 5512	O AS CB AS CG AS OD1 AS		710 710 710 710	4 4 4 4	8.946 7.907 9.694 9.111 9.565	56.073 55.862 56.693 55.457 55.108	41.930 42.499 39.529 38.877 37.760	1.00 1.00 1.00 1.00	22.19 23.72 25.68
70	ATOM ATOM ATOM ATOM	5513 5514 5515 5516	CA V	SN A L A L A L A	711 711	5 5	8.155 0.057 0.087 0.699	54.793 55.420 54.473 55.297	39.503 42.238 43.350 44.466	1.00 : 1.00 : 1.00 :	20.50 23.96 23.22

	ATOM	5517	0	VAL A		51.873	55.501	44.452	1.00 22.80
	ATOM	5518	CB	VAL A		50.972	53.283	43.047	1.00 22.97
	ATOM	5519	CG1	VAL A	711	51.160	52.431	44.299	1.00 23.01
	ATOM	5520	CG2	VAL A		50.368	52.450	41.924	1.00 23.83
5	MOTA	5521	N	HIS A		49.904	55.814	45.400	1.00 22.89
	ATOM	5522	CA	HIS A		50.416	56.834	46.359	1.00 21.66
	ATOM	5523	С	HIS A		51.501	56.353	47.274	1.00 21.27
	ATOM	5524	0	HIS A		51.530	55.188	47.648	1.00 21.83
	MOTA	5525	CB	HIS A		49.277	57.418	47.149	1.00 21.88
10	MOTA	5526	CG	HIS A		48.215	57.987	46.295	1.00 21.78
	ATOM	5527		HIS A		46.879	57.853	46.585	1.00 23.44
	MOTA	5528		HIS A		48.288	58.645	45.111	1.00 24.89
	ATOM	5529		HIS A		46.172	58.414	45.617	1.00 26.25
	ATOM	5530	NE2			47.002	58.900	44.710	1.00 23.73
15	MOTA	5531	N	PHE A		52.434	57.241	47.602	1.00 21.76
	ATOM	5532	CA	PHE A		53.548	56.891	48.497	1.00 21.66
	ATOM	5533	C	PHE A		52.955	56.240	49.755	1.00 21.63
	ATOM	5534	0_	PHE A		53.514	55.305	50.331	1.00 21.09
	ATOM	5535	CB	PHE A		54.376	58.127	48.822	1.00 21.67
20	ATOM	5536	CG	PHE A		55.544	57.844	49.691	1.00 22.98
	ATOM	5537		PHE A		56.709	57.363	49.148	1.00 23.95
	ATOM	5538	CD2		713	55.464	58.032	51.068	1.00 23.46
	MOTA	5539	CE1			57.761	57.053	49.962	1.00 24.01
	ATOM	5540	CE2			56.543	57.743	51.890	1.00 24.07
25	ATOM	5541	CZ	PHE A		57.680	57.269	51.347	1.00 22.72
	ATOM	5542	N	GLN A		51.801	56.747	50.153	1.00 21.89
	ATOM	5543	CA	GLN A		50.999	56.145	51.221	1.00 21.58
	ATOM	5544	C	GLN A		51.062	54.650	51.275	1.00 21.88 1.00 21.77
20	ATOM	5545	O	GLN A		51.122	54.049 56.516	52.353	
30	ATOM	5546	CB	GLN A GLN A		49.530 48.521	55.708	50.996 51.846	1.00 22.22 1.00 22.39
	ATOM	5547 5548	CG	GLN A		47.083	55.934	51.412	1.00 25.35
	ATOM	5549	CD OE1			46.801	56.149	50.215	1.00 23.33
	ATOM ATOM	5550	NE2			46.162	55.906	52.385	1.00 19.33
35	ATOM	5551	NEZ	GLN A		50.991	54.021	50.111	1.00 24.01
33	ATOM	5552	CA	GLN A		50.863	52.567	50.098	1.00 22.47
	ATOM	5553	C	GLN A		52.113	51.959	50.686	1.00 21.96
	ATOM	5554	ŏ	GLN A		52.039	51.017	51.456	1.00 21.62
	ATOM	5555	ČВ	GLN A	715	50.590	52.006	48.671	1.00 23.33
40	ATOM	5556	CG	GLN A		49.484	52.714	47.865	1.00 22.85
	ATOM	5557	CD	GLN A		48.460	51.803	47.206	1.00 23.26
	ATOM	5558	OE1			47.763	52.237	46.256	1.00 26.33
	ATOM	5559	NE2		715	48.357	50.553	47.672	1.00 21.21
	ATOM	5560	N	SER A	716	53.282	52.477	50.312	1.00 21.68
45	ATOM	5561	CA	SER A	716	54.535	51.955	50.865	1.00 21.21
	ATOM	5562	С	SER A	716	54.790	52.436	52.288	1.00 21.13
	ATOM	5563	0	SER A	716	55.427	51.732	53.076	1.00 21.25
	ATOM	5564	CB	SER A	716	55.724	52.393	50.028	1.00 20.77
	MOTA	5565	OG	SER A	716	55.750	51.785	48.782	1.00 22.33
50	MOTA	5566	N	ALA A	717	54.341	53.643	52.613	1.00 20.84
	MOTA	5567	CA	ALA A	717	54.434	54.129	54.003	1.00 21.57
	ATOM	5568	С	ALA A	717	53.702	53.210	54.988	1.00 21.28
	MOTA	5569	0	ALA A		54.114	53.054	56.120	1.00 21.81
	ATOM	5570	CB		717	53.879	55.507	54.103	1.00 21.20
55	ATOM	5571	N	GLN A	718	52.609	52.606	54.534	1.00 21.73
	ATOM	5572	CA		718	51.833	51.680	55.345	1.00 20.77
	ATOM	5573	С	GLN A		52.543	50.336	55.332	1.00 22.09
	MOTA	5574	0	GLN A		52.531	49.610	56.321	1.00 21.08
	MOTA	5575	CB	GLN A	718	50.398	51.579	54.843	1.00 20.57
60	MOTA	5576	CG	GLN A		49.534	52.822	55.036	1.00 19.42
	MOTA	5577	CD	GLN A	718	49.086	53.107	56.516	1.00 21.11
	ATOM	5578		GLN A	718	49.500	52.423	57.442	1.00 20.25
	MOTA	5579	NE2		718	48.233	54.128	56.700	1.00 19.84
<i>-</i> -	ATOM	5580	N	ILE A	719	53.220	49.980	54.230	1.00 23.16
65	ATOM	5581	CA	ILE A	719	54.015	48.754	54.294	1.00 23.10
	ATOM	5582	C	ILE A	719	55.157	48.879	55.323	1.00 23.04
	ATOM	5583	0	ILE A		55.402	47.996	56.111	1.00 21.76
	MOTA	5584	CB	ILE A	719	54.618	48.352	52.972	1.00 23.18
70	ATOM	5585	CG1			53.513	47.935	52.000	1.00 24.68
70	ATOM	5586	CG2	ILE A	119	55.536	47.183	53.202	1.00 23.59

5	ATOM ATOM ATOM ATOM ATOM ATOM	5587 5588 5589 5590 5591 5592 5593	N CA C O CB OG	SER A SER A SER A SER A SER A	720 720 720 720 720 720 720	54.013 55.894 57.033 56.568 57.156 57.801	49.966 50.144 50.144 49.515 51.421 52.588	50.705 55.254 56.140 57.604 58.470 55.759 56.142	1.00 1.00 1.00 1.00	
10	ATOM ATOM ATOM ATOM ATOM	5594 5595 5596 5597 5598	N CA C O CB	LYS A LYS A LYS A LYS A LYS A	721 721 721 721	55.476 55.037 54.591 54.776 53.910	50.922 49.594	57.878 59.238 59.802 61.013 59.355	1.00 1.00 1.00	23.57 23.10 23.13 22.76
15	ATOM ATOM ATOM ATOM	5599 5600 5601 5602 5603	CG CD CE NZ N	LYS A LYS A LYS A LYS A ALA A	721 721 721 722	53.364 52.518 51.164 50.635 54.045	52.005 53.195 52.901 54.174 48.741	60.767 60.884 60.264 59.874 58.942	1.00 1.00 1.00	26.29 28.49 29.77 21.71
20	ATOM ATOM ATOM ATOM	5604 5605 5606 5607 5608	CA C O CB N	ALA A ALA A ALA A LEU A	722 722 722 723	53.639 54.871 54.842 52.657 55.942	47.437 46.531 45.733 46.800 46.652	59.407 59.693 60.629 58.432 58.922	1.00 1.00 1.00	21.58 21.73 22.32 21.13
25	ATOM ATOM ATOM ATOM ATOM	5609 5610 5611 5612 5613	CA C O CB CG	LEU A	723 723 723 723	57.132 57.833 58.415 58.108 57.581	45.849 46.308 45.510 45.903 45.424	59.176 60.477 61.161 57.981 56.608	1.00 1.00 1.00	22.59 23.17 23.51 22.95 25.06
30	ATOM ATOM ATOM ATOM ATOM	5614 5615 5616 5617 5618		LEU A LEU A VAL A VAL A VAL A	723 724 724	58.559 57.321 57.749 58.296 57.515	45.715 43.963 47.605 48.200 47.720	55.470 56.630 60.778 62.001 63.211	1.00 1.00 1.00	25.60 26.11 25.38 26.75 27.37
35	ATOM ATOM ATOM ATOM ATOM	5619 5620 5621 5622 5623	O CB CG1 CG2 N	VAL A VAL A VAL A VAL A ASP A	724 724 724	58.121 58.306 58.535 59.370 56.185	47.337 49.765 50.414 50.244 47.729	64.192 61.944 63.349 60.938	1.00 1.00 1.00 1.00	25.90 26.41 26.97 27.86
40	ATOM ATOM ATOM ATOM ATOM	5624 5625 5626 5627 5628	CA C O CB CG	ASP A ASP A ASP A ASP A ASP A	725 725 725 725	55.358 55.558 55.224 53.866 53.522	47.729 47.253 45.775 45.321 47.502 48.994	63.144 64.271 64.575 65.672 64.029 63.937	1.00 1.00 1.00 1.00	29.06 30.17 30.11 30.77 31.42 34.46
45	ATOM ATOM ATOM ATOM ATOM	5629 5630 5631 5632 5633	OD1	ASP A ASP A VAL A VAL A VAL A	725 725 726 726	54.308 52.471 56.101 56.341	49.854 49.377 45.012 43.590	64.410 63.418 63.640 63.901	1.00 1.00 1.00 1.00	36.27 36.23 29.60 30.28
50	ATOM ATOM ATOM ATOM ATOM	5634 5635 5636 5637 5638	O CB CG1	VAL A VAL A VAL A VAL A GLY A	726 726 726 726	57.861 58.249 55.626 56.253 54.135 58.723	43.262 42.117 42.761 41.453 42.552 44.277	64.099 64.275 62.768 62.563 63.096 64.124	1.00 1.00 1.00 1.00	30.42 31.01 31.65 36.09 31.33 29.48
55	ATOM ATOM ATOM ATOM ATOM	5639 5640 5641 5642 5643	CA C O N CA	GLY A GLY A GLY A VAL A VAL A	727 727 727 728	60.150 60.860 61.785 60.464 61.109	44.064 43.434 42.644 43.775 43.125	64.297 63.102 63.272 61.869 60.737	1.00	28.80 28.95 26.93 29.03
60	ATOM ATOM ATOM ATOM ATOM	5644 5645 5646 5647	C O CB CG1	VAL A VAL A VAL A	728 728 728 728	62.058 61.684 60.082 60.754	44.099 45.196 42.672 42.337	60.160 59.883 59.639 58.345	1.00 1.00 1.00 1.00	27.94 27.99 29.59 29.88
65	ATOM ATOM ATOM ATOM ATOM	5648 5649 5650 5651 5652 5653	N CA C O	VAL A ASP A ASP A ASP A ASP A ASP A	729 729 729 729	59.350 63.309 64.223 64.138 63.759 65.622	41.464 43.736 44.677 44.520 43.476 44.432	60.091 59.986 59.377 57.832 57.362 59.885	1.00 1.00 1.00 1.00 1.00	28.23 29.21 29.09 29.53
70	ATOM ATOM ATOM	5654 5655 5656	CG OD1	ASP A TASP A TASP A	729 729	66.604 66.262 67.772	45.518 46.732 45.225	59.439 59.395 59.140	1.00 1.00 1.00	32.15 30.16

	ATOM	5657	N	PHE A	730	64.433	45.575	57.088	1.00	28.48
	ATOM	5658	CA	PHE A		64.397	45.571	55.627	1.00	
	ATOM	5659	С	PHE A		65.099	46.820	55.186	1.00	
	ATOM	5660	0	PHE A	730	65.429	47.666	56.012	1.00	28.30
5	ATOM	5661	CB	PHE A	730	62.965	45.646	55.103	1.00	28.89
-	ATOM	5662	CG	PHE A		62.222	46.857	55.585	1 00	27.56
	MOTA	5663	CD1			61.704	46.895	56.851	1.00	
	ATOM	5664	CD2	PHE A	730	62.081	47.960	54.788	1.00	28.64
	ATOM	5665	CE1	PHE A	730	61.031	48.016	57.316	1.00	25.09
10						61.424	49.083	55.247		28.36
10	ATOM	5666	CE2							
	ATOM	5667	cz	PHE A	730	60.895	49.098	56.528	1.00	27.46
	ATOM	5668	N	GLN A	731	65.298	46.966	53.889	1.00	28.36
	ATOM	5669	CA	GLN A	731	65.953	48.144	53.363	1.00	29.43
							48.998			
	ATOM	5670	C	GLN A		64.909		52.632	1.00	
15	ATOM	5671	0	GLN A	731	63.884	48.482	52.143	1.00	29.07
	ATOM	5672	CB	GLN A	731	67.110	47.739	52.447	1.00	29.69
	ATOM	5673	ĊĠ	GLN A		68.266	46.944	53.180		34.65
	MOTA	5674	CD	GLN A		69.065	46.054	52.228		39.33
	ATOM	5675	OE1	GLN A	731	69.361	44.845	52.519	1.00	40.43
20	ATOM	5676	NE2	GLN A	731	69.438	46.638	51.089	1.00	40.02
				ALA A		65.217	50.285	52.493	1.00	
	ATOM	5677	N							
	ATOM	5678	CA	ALA A		64.301	51.224	51.903	1.00	28.92
	ATOM	5679	С	ALA A	732	64.989	52.315	51.072	1.00	28.18
	ATOM	5680	0	ALA A		66.126	52.630	51.271	1.00	28.14
25								52.975		29.05
25	ATOM	5681	CB	ALA A		63.538	51.875			
	ATOM	5682	N	MET A	733	64.228	52.947	50.208	1.00	26.98
	ATOM	5683	CA	MET A	733	64.705	54.082	49.478	1.00	26.14
	ATOM	5684	C	MET A		63.474	54.827	48.990	1 00	25.35
	-									
	ATOM	5685	0	MET A		62.614	54.253	48.296		25.39
30	ATOM	5686	CB	MET A	733	65.527	53.651	48.288	1.00	25.92
	ATOM	5687	CG	MET A	733	65.990	54.829	47.411	1.00	28.55
	ATOM	5688	SD	MET A		67.202	55.830	48.257	1.00	31.06
	MOTA	5689	CE	MET A	733	68.354	54.472	48.738		30.06
	ATOM	5690	N	TRP A	734	63.368	56.086	49.369	1.00	24.30
35	ATOM	5691	CA	TRP A	734	62.312	56.941	48.858	1.00	23.89
	ATOM	5692	C	TRP A	734	62.965	57.750	47.759		23:75
	ATOM	5693	0	TRP A	734	64.171	57.880	47.786	1.00	
	ATOM	5694	CB	TRP A	734	61.799	57.833	49.974	1.00	23.65
	MOTA	5695	CG	TRP A	734	62.719	58.977	50.358	1.00	21.94
40	ATOM	5696	CD1			62.863	60.139	49.699		20.95
40			_							
	ATOM	5697	CD2	TRP A		63.542	59.079	51.523		19.59
	ATOM	5698	NE1	TRP A	734	63.763	60.954	50.351	1.00	21.98
	ATOM	5699	CE2	TRP A	734	64.177	60.328	51.485	1.00	19.47
	ATOM	5700	CE3	TRP A	734	63.808	58.243	52.602		19.81
4-										
45	ATOM	5701	CZ2	TRP A	734	65.064	60.745	52.455		20.40
	MOTA	5702	CZ3	TRP A	734	64.723	58.649	53.554		19.84
	MOTA	5703	CH2	TRP A	734	65.316	59.894	53.490	1.00	21.63
	ATOM	5704		TYR A		62.228				23.61
	ATOM	5705	CA	TYR A		62.867	59.074	45.731		24.11
50	MOTA	5706	С	TYR A	735	62.082	60.358	45.708		23.54
	ATOM	5707	0	TYR A	735	60.917	60.392	45.252	1.00	22.73
	ATOM	5708	СB	TYR A		62.927	58.420	44.330		23.78
	ATOM	5709	CG	TYR A		64.078	57.476	44.193		23.59
	ATOM	5710	CD1	TYR A	735	65.335	57.942	43.903	1.00	23.44
55	MOTA	5711	CD2	TYR A	735	63.916	56.122	44.371	1.00	23.85
	ATOM	5712		TYR A		66.396	57.103	43.822		22.40
	MOTA	5713		TYR A		64.984	55.276	44.305		26.43
	ATOM	5714	CZ	TYR A		66.235	55.784	44.016	1.00	25.37
	ATOM	5715	OH	TYR A	735	67.325	54.958	43.938		24.12
60	MOTA	5716	N	THR A		62.729	61.425	46.174		23.46
JU										
	MOTA	5717	CA	THR A		62.009	62.673	46.288		22.55
	ATOM	5718	С	THR A	736	61.636	63.356	45.010	1.00	23.03
	ATOM	5719	ō	THR A		62.434	63.507	44.094		22.95
	MOTA	5720	СВ	THR A		62.527	63.627	47.410		23.38
65	MOTA	5721		THR A		62.759	64.943	46.931		19.53
	ATOM	5722	CG2	THR A	736	63.748	63.165	48.096	1.00	21.12
	ATOM	5723	N	ASP A		60.341	63.678	44.976		23.42
	MOTA	5724	CA	ASP A		59.642	64.375	43.929		23.60
	ATOM	5725	С	ASP A	737	59.514	63.537	42.632	1.00	24.09
70	MOTA	5726	0	ASP A		59.127	64.055	41.586	1.00	25.66
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SER A 745
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69.584
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65
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70
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                     C
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                                                                 38.747
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5	ATOM ATOM ATOM ATOM ATOM ATOM	5797 5798 5799 5800 5801 5802 5803	O CB N CA C O CB	ALA HIS	A A A A	748	66.85 65.15 66.31 66.32 67.71 67.85 65.99	9 59.3 9 57.5 3 56.2 2 55.6 7 54.4	98 39.692 13 37.451 21 36.779 01 36.943 44 37.288	1.00 1.00 1.00 1.00	28.23 27.13 26.90 25.91 24.98 24.25 26.95
10	ATOM ATOM ATOM ATOM ATOM	5804 5805 5806 5807 5808	CG ND1 CD2 CE1 NE2	HIS HIS HIS HIS	A A A A	748 748 748 748 748	66.17 65.21 67.19 65.64 66.85	55.23 55.23 54.29 8 54.83 4 53.29 53.63	34.452 34.345 29 33.660 99 33.540 20 33.119	1.00 1.00 1.00 1.00	26.97 26.07 30.08 30.19 28.24
15	ATOM ATOM ATOM ATOM ATOM ATOM	5809 5810 5811 5812 5813 5814	N CA C O CB CG	GLN GLN GLN GLN GLN GLN	A A A A	749 749 749 749 749	68.75 70.10 70.35 70.89 71.15 71.04	9 55.82 0 55.3 0 54.29 6 56.84 7 57.23	36.866 78 38.323 95 38.603 18 36.423 12 34.965	1.00 1.00 1.00 1.00	24.83 24.85 23.61 21.42 25.62 28.72
20	ATOM ATOM ATOM	5815 5816 5817 5818	CD OE1 NE2 N		A A	749 749	72.02 73.22 71.52 69.83	0 58.03 4 59.49	34.446 34.295	$1.00 \\ 1.00$	35.38 40.06 36.86 22.63
25	ATOM ATOM ATOM ATOM ATOM	5819 5820 5821 5822 5823	CA C O CB CG	HIS HIS HIS HIS	A A A	750 750 750	70.11 69.34 69.90 69.96 70.30	0 54.67 9 53.83 6 57.14	75 41.143 44 41.764 18 41.492	1.00 1.00 1.00	24.02 22.54 23.89 24.83 27.84
30	ATOM ATOM ATOM ATOM	5824 5825 5826 5827	ND1 CD2 CE1	HIS HIS HIS	A A A	750 750 750 750	71.26 69.81 71.34 70.48	3 57.70 2 56.10 3 57.33 5 56.34	05 43.572 04 43.863 02 44.837 18 45.034	1.00 1.00 1.00 1.00	30.28 28.68 27.63 28.75
35	ATOM ATOM ATOM ATOM ATOM	5828 5829 5830 5831 5832	N CA C O CB	ILE ILE ILE ILE	A A A	751 751 751	68.07 67.35 67.92 68.00 65.84	5 53.32 0 52.02 4 51.03	41.292 40.729 7 41.442	1.00 1.00 1.00	23.23 22.24 23.39 23.47 21.86
40	ATOM ATOM ATOM ATOM	5833 5834 5835 5836	CG1 CG2 CD1	ILE ILE ILE TYR	A A A	751 751	65.05 65.52 63.49 68.25	7 52.35 6 53.26 0 52.44	41.771 39.575 7 41.548	1.00 1.00 1.00	21.82 21.39 22.67 23.82
10	ATOM ATOM ATOM ATOM	5837 5838 5839 5840	CA C O CB	TYR TYR TYR TYR	A A A	752 752 752	68.77 70.15 70.53 68.73	1 50.71 4 50.41 8 49.27	6 38.890 7 39.436 6 39.554	1.00 1.00 1.00	24.50 23.94 24.99 24.24
45	ATOM ATOM ATOM ATOM	5841 5842 5843 5844	CG CD1 CD2 CE1	TYR TYR	A A A	752 752 752	67.34 66.89 66.49 65.66	8 50.33 5 49.02 1 51.31	5 36.850 1 36.863 0 36.418	1.00 1.00 1.00	24.42 25.36 23.66 26.62
50	ATOM ATOM ATOM ATOM	5845 5846 5847 5848	CE2 CZ OH N	TYR TYR TYR THR	A A A	752 752 752	65.23 64.82 63.55 70.88	0 50.99 3 49.67 2 49.34	6 35.993 9 35.983 1 35.576	1.00	26.62 27.74 31.07
55	ATOM ATOM ATOM ATOM	5849 5850 5851 5852	CA C O CB	THR THR THR THR	A A A A	753 753 753 753	72.18 72.00 72.63 72.94	0 51.26 3 50.68 4 49.70 8 52.62	6 40.416 9 41.809 6 42.159 0 40.431	1.00 1.00 1.00	24.64 24.38 24.12 25.26
60	ATOM ATOM ATOM ATOM ATOM	5853 5854 5855 5856	OG1 CG2 N CA	THR THR HIS HIS	A A A	753 754 754	73.15 74.34 71.06 70.83	52.46 51.23 50.75	8 40.989 5 42.571 3 43.940	1.00 1.00 1.00	24.69 25.36 25.62
65	ATOM ATOM ATOM ATOM	5857 5858 5859 5860 5861	C O CB CG ND1	HIS HIS HIS	A A A	754 754 754	70.29 70.69 69.85 69.94 71.10	4 48.47 5 51.66 8 51.63	8 44.673 7 44.667 1 46.158		24.87
	ATOM ATOM ATOM ATOM	5862 5863 5864 5865	CD2 CE1	HIS HIS HIS MET	A A A	754 754 754	69.01 70.87 69.62 69.38	2 51.34 7 51.80 0 51.44	9 47.101 7 48.146 3 48.320	1.00 1.00 1.00	29.11 32.00
70	ATOM	5866	CA	MET	A	755	68.80	7 47.75	3 42.904	1.00	24.59

	ATOM ATOM	5867 5868	_		A 755 A 755	69.860 69.820			
	ATOM	5869	_		A 755	67.606	47.727		
	ATOM	5870			A 755	66.364	48.479		
5		5871	. SD		A 755	64.919	48.067		
	ATOM	5872			A 755	65.463	48.670	39.959	1.00 29.78
	ATOM	5873			A 756	70.809	47.118		
	ATOM ATOM	5874 5875			A 756	71.831	46.155	41.172	
10		5876			A 756 A 756	72.724 72.988	45.760	42.352	
	ATOM	5877	_		A 756	72.701	44.568 46.723	42.559 40.043	1.00 26.03 1.00 26.64
	ATOM	5878			A 756	71.911	47.057	38.918	1.00 28.16
	ATOM	5879	N	HIS	A 757	73.171	46.750	43.139	1.00 27.24
	MOTA	5880		HIS		73.969	46.437	44.313	1.00 27.68
15	ATOM	5881	_		A 757	73.222	45.445	45.171	1.00 27.98
	ATOM ATOM	5882 5883	_		A 757	73.808	44.452	45.642	1.00 28.11
	ATOM	5884	CB CG		A 757 A 757	74.315 75.311	47.685	45.147	1.00 28.80
	ATOM	5885		HIS		76.438	48.605 48.146	44.489 43.838	1.00 29.61 1.00 34.38
20	MOTA	5886		HIS		75.363	49.956	44.418	1.00 34.38
	ATOM	5887		HIS		77.124	49.177	43.370	1.00 36.17
	MOTA	5888		HIS.		76.493	50.289	43.715	1.00 33.47
	ATOM	5889	N		A 758	71.915	45.649	45.335	1.00 27.26
25	ATOM ATOM	5890 5891	CA C		A 758 A 758	71.140	44.810	46.240	1.00 26.79
23	ATOM	5892	0		A 758 A 758	71.021 71.187	43.381 42.438	45.735	1.00 28.64
	ATOM	5893	СВ		A 758	69.771	45.447	46.508 46.514	1.00 28.71 1.00 26.31
	ATOM	5894	CG		A 758	68.874	44.611	47.374	1.00 25.31
	ATOM	5895	CD1	PHE	A 758	68.008	43.691	46.801	1.00 24.16
30		5896		PHE 2		68.868	44.753	48.753	1.00 24.21
	ATOM	5897		PHE 2		67.143	42.914	47.595	1.00 23.28
	ATOM ATOM	5898 5899	CE2	PHE A	A 758 A 758	68.015	43.957	49.547	1.00 25.66
	ATOM	5900	N		A 759	67.164 70.771	43.030 43.186	48.943 44.442	1.00 25.26
35	ATOM	5901	CA	ILE A		70.711	41.827	43.920	1.00 29.59 1.00 30.59
	ATOM	5902	C	ILE A	A 759	72.091	41.168	44.009	1.00 30.33
	ATOM	5903	0	ILE A		72.204	39.986	44.386/	1.00 30.69
	ATOM	5904	CB	ILE A	A 759	70.215	41.816	42.465	1.00 31.21
40	ATOM ATOM	5905 5906		ILE A		68.740	42.175	42.397	1.00 33.66
40	ATOM	5907	CD1	ILE A	1 759	70.465 67.781	40.451 41.070	41.860 43.005	1.00 33.00
	ATOM	5908	N	LYS A		73.140	41.070	43.668	1.00 35.66 1.00 32.46
	MOTA	5909	CA	LYS A		74.514	41.392	43.708	1.00 32.40
	ATOM	5910	С	LYS A	760	74.896	40.871	45.109	1.00 34.58
45	ATOM	5911	0	LYS A		75.415	39.770	45.248	1.00 35.10
	ATOM ATOM	5912 5913	CB	LYS A		75.523	42.433	43.174	1.00 33.78
	ATOM	5914	CG CD	LYS A		75.359	42.680	41.645	1.00 35.41
	ATOM	5915	CE	LYS A		77.512	42.011	40.894	1.00 37.74 1.00 39.01
50	ATOM	5916	NZ	LYS A		78.711	44.128	40.596	1.00 39.64
	ATOM	5917	N	GLN A	761	74.573	41.612	46.160	1.00 35.44
	ATOM	5918	CA	GLN A		74.928	41.152	47.495	1.00 35.72
	ATOM	5919	C	GLN A		74.048	40.003	47.970	1.00 36.14
55	ATOM ATOM	5920 5921	O CB	GLN A		74.552	39.051	48.584	1.00 34.84
55	ATOM	5922	CG	GLN A		74.992 73.719	42.308 42.855	48.476 48.947	1.00 36.42 1.00 39.46
	ATOM	5923	CD	GLN A		73.014	41.956	49.923	1.00 39.46
	MOTA	5924	OE1			73.652	41.146	50.597	1.00 47.15
	ATOM	5925	NE2	GLN A	761	71.669	42.072	49.987	1.00 46.69
60	ATOM	5926	Ŋ	CYS A		72.765	40.013	47.599	1.00 36.07
	ATOM	5927	CA	CYS A		71.921	38.898	47.934	1.00 37.51
	ATOM ATOM	5928 5929	C O	CYS A		72.395 72.158	37.625	47.229	1.00 37.30
	ATOM	5930	CB	CYS A		72.158 70.457	36.518 39.208	47.728	1.00 37.19
65	ATOM	5931	SG	CYS A		69.317	39.208	47.609 47.558	1.00 37.88 1.00 43.96
	ATOM	5932	N	PHE A		73.053	37.773	46.076	1.00 43.36
	MOTA	5933	CA	PHE A	763	73.506	36.622	45.313	1.00 37.34
	ATOM	5934	C	PHE A		74.982	36.320	45.533	1.00 38.08
70	ATOM ATOM	5935 5936	O	PHE A			35.436	44.902	1.00 37.30
, 0	AIUM	5936	СВ	PHE A	103	73.242	36.832	43.818	1.00 37.64

	ATOM	5937	CG	PHE	Α	763	71.803	36.621	43.415	1.00 37.37
	ATOM	5938	CD1				70.904	36.029	44.274	1.00 34.64
	ATOM	5939	CD2				71.349	37.052	42.189	1.00 36.85
	ATOM	5940	CE1				69.611	35.850	43.907	1.00 33.81
5	ATOM	5941	CE2	PHE			70.032	36.872	41.828	1.00 35.30
,		5942	CZ	PHE			69.176	36.272	42.691	1.00 33.56
	ATOM						75.606	37.034		1.00 33.30
	ATOM	5943	N	SER				_	46.467	
	ATOM	5944	CA	SER			77.031	36.880	46.818	1.00 41.43
	ATOM	5945	C	SER			77.910	37.043	45.578	1.00 42.27
10	ATOM	5946	0	SER			78.843	36.274	45.374	1.00 42.04
	ATOM	5947	СВ	SER			77.315	35.531	47.502	1.00 41.77
	ATOM	5948	OG	SER			76.407	35.254	48.579	1.00 41.18
	ATOM	5949	N	LEU			77.587	38.058	44.772	1.00 42.51
	ATOM	5950	CA	LEU	Α	765	78.294	38.354	43.535	1.00 43.43
15	ATOM	5951	С	LEU	Α	765	79.064	39.660	43.666	1.00 44.05
	ATOM	5952	0	LEU	Α	765	78.499	40.660	44.070	1.00 43.63
	ATOM	5953	CB	LEU	Α	765	77.307	38.511	42.357	1.00 42.63
	ATOM	5954	CG	LEU	Α	765	76.470	37.312	41.885	1.00 43.40
	ATOM	5955	CD1	LEU	Α	765	75.445	37.749	40.818	1.00 42.42
20	ATOM	5956	CD2	LEU	Α	765	77.358	36.214	41.312	1.00 44.39
	ATOM	5957	N	PRO			80.352	39.649	43.334	1.00 45.52
	ATOM	5958	CA	PRO			81.149	40.878	43.291	1.00 46.31
	ATOM	5959	C	PRO			80.972	41.528	41.939	1.00 47.02
	ATOM	5960	ŏ	PRO			80.814	40.744	40.984	1.00 48.05
25	ATOM	5961	ČВ	PRO			82.582	40.368	43.425	1.00 46.75
	ATOM	5962	CG	PRO			82.441	38.840	43.696	1.00 46.59
	ATOM	5963	CD	PRO			81.168	38.462	43.016	1.00 45.98
	TER	5964	CD	PRO			01.100	30.402	43.010	1.00 43.50
	HETATM		C1	NAG			52.247	84.441	26.665	1.00 56.57
30	HETATM		C2	NAG			51.667	85.774	26.181	1.00 59.26
30				NAG			50.405	85.614	25.454	1.00 59.20
	HETATM		N2							1.00 63.64
	HETATM		C7	NAG			50.230	84.786	24.417	
	HETATM		07	NAG			49.104	84.445	24.028	1.00 64.39
25	HETATM		C8	NAG			51.434	84.255	23.678	1.00 63.71
35	HETATM		C3	NAG			52.732	86.604	25.440	1.00 59.62
	HETATM		03	NAG			52.304	87.904	25.060	1.00 59.46
	HETATM		C4	NAG			53.931	86.799	26.333	1.00 59.23
	HETATM		04	NAG			54.958	87.354	25.538	1.00 58.87
	HETATM		C5	NAG			54.379	85.491	26.977	1.00 58.73
40	HETATM		C6	NAG			55.422	85.799	28.061	1.00 58.77
	HETATM		06	NAG			54.806	86.202	29.259	1.00 58.36
	HETATM	5978	05	NAG	Α	793	53.306	84.773	27.544	1.00 56.72
	HETATM	5979	C1	NAG			57.357	62.419	-5.828	1.00 28.91
	HETATM	5980	C2	NAG	Α	794	57.044	63.800	-5.253	1.00 30.20
45	HETATM	5981	N2	NAG	Α	794	56.632	63.635	-3.866	1.00 29.11
	HETATM	5982	C7	NAG	Α	794	57.358	63.964	-2.815	1.00 29.67
	HETATM	5983	07	NAG			58.514	64.379	-2.847	1.00 28.47
	HETATM	5984	C8	NAG	Α	794	56.666	63.783	-1.481	1.00 30.86
	HETATM	5985	C3	NAG	Α	794	55.889	64.431	-6.033	1.00 31.06
50	HETATM		03	NAG			55.644	65.736	-5.613	1.00 32.22
	HETATM		C4	NAG			56.322	64.529	-7.468	1.00 32.03
	HETATM		04	NAG			55.313	65.150	-8.198	1.00 30.75
	HETATM		C5	NAG			56.558	63.108	-7.965	1.00 32.35
	HETATM		C6	NAG			56.903	63.109	-9.455	1.00 32.88
55	HETATM		06	NAG			57.858	64.097	-9.728	1.00 30.65
	HETATM		05	NAG			57.632	62.574	-7.216	1.00 31.57
	HETATM		C1	NAG			26.557	83.475	27.320	1.00 69.38
	HETATM		C2	NAG			26.517	84.675	28.278	1.00 70.37
	HETATM		N2	NAG			27.031	85.876	27.627	1.00 71.29
60	HETATM		C7	NAG			26.337	86.484	26.653	1.00 72.14
50				NAG			25.108	86.415	26.530	1.00 72.14
	HETATM		07 C8	NAG				87.272	25.659	1.00 71.13
	HETATM		C8				27.135		29.631	
	HETATM		C3	NAG			27.147	84.328		1.00 68.73
6	HETATM		03	NAG			27.036	85.420	30.524	1.00 67.24
65	HETATM		C4	NAG			26.366	83.126	30.165	1.00 68.79
	HETATM		04	NAG			26.805	82.703	31.436	1.00 65.52
	HETATM		C5	NAG			26.453	81.990	29.151	1.00 70.52
	HETATM	6004	C6	NAG			25.734	80.729	29.625	1.00 71.77
	HETATM		06	NAG			25.527	79.863	28.524	1.00 71.65
70	HETATM	6006	05	NAG	Α	795	25.881	82.386	27.919	1.00 70.37

5	HETAT HETAT HETAT HETAT	M 6007 M 6008 M 6009 M 6010 M 6011 M 6012	C2 N2 C7	NAG A NAG A	A 796 A 796 A 796 A 796 A 796	28.778 27.615 28.001 27.907 27.527 28.341	70.692 71.731 71.604 70.594	39.410 38.471 37.160	1.00 35.69 1.00 33.86 1.00 34.06 1.00 36.08
10	HETAT HETAT HETAT HETAT HETAT HETAT	M 6013 M 6014 M 6015 M 6016 M 6017 M 6018	C3 O3 C4 O4 C5 C6	NAG A	A 796 A 796 A 796 A 796 A 796	27.015 25.98 26.563 26.063 27.784 27.444	71.446 72.255 70.490 71.140 69.659	40.578 40.072 41.666 42.848 42.014 43.129	
15		M 6019 M 6020 6021 6022 6023 6024	05	NAG A NAG A SER E SER E SER E	796 3 39 3 39 3 39	26.267 28.232 83.809 82.610 81.248 80.264	68.081 68.954 35.290 34.403 35.137	42.668 40.876 81.108 81.141 81.269	1.00 44.11 1.00 33.47 1.00 44.51 1.00 44.41 1.00 44.06
20	ATOM ATOM ATOM ATOM	6025 6026 6027 6028	CB · OG N CA	SER E SER E ARG E	3 39 3 39 3 40 3 40	82.751 81.500 81.151 79.877	33.364 32.762 36.191 36.926	80.681 82.277 82.630 82.082 82.188	1.00 44.10 1.00 44.82 1.00 44.84 1.00 43.21 1.00 42.08
25	ATOM ATOM ATOM ATOM ATOM	6029 6030 6031 6032	C O CB CG CD	ARG E ARG E ARG E ARG E	40 40 40	79.254 79.926 80.006 80.757 82.151	37.440 38.223 38.172	80.843 79.822 83.002 84.357 84.248	1.00 40.45 1.00 39.04 1.00 42.78 1.00 43.26 1.00 45.08
30	ATOM ATOM ATOM ATOM ATOM	6034 6035 6036 6037 6038	NE CZ NH1	ARG B ARG B ARG B ARG B LYS B	40 40 40 40	82.289 83.237 84.100 83.318 77.947	40.180	84.761 84.357 83.413 84.868 80.852	1.00 46.19 1.00 47.79 1.00 49.11 1.00 49.15
35	ATOM ATOM ATOM ATOM	6039 6040 6041 6042	CA C O CB	LYS B LYS B LYS B	41 41 41 41	77.314 77.790 78.326 75.796	38.071 39.496 40.226 38.000	79.643 79.349 80.180 79.712	1.00 39.26 1.00 38.31 1.00 36.90 1.00 36.21 1.00 38.22
40	ATOM ATOM ATOM ATOM ATOM	6043 6044 6045 6046 6047	CG CD CE NZ N	LYS B LYS B LYS B LYS B THR B	41 41 41 41 42	75.166 73.659 72.987 73.185 77.593	38.814 38.723 40.028 40.341 39.860	80.815 80.787 80.320 78.870 78.118	1.00 39.94 1.00 42.54 1.00 44.09 1.00 43.20 1.00 35.87
45	ATOM ATOM ATOM ATOM ATOM	6048 6049 6050 6051 6052	CA C O CB OG1		42 42 42 42 42	77.981 76.658 75.604 78.542 79.892	41.136 41.941 41.329 40.805 41.260	77.584 77.535 77.564 76.215 76.064	1.00 35.53 1.00 33.81 1.00 34.18 1.00 36.04 1.00 38.02
50	ATOM ATOM ATOM ATOM ATOM	6053 6054 6055 6056 6057	CG2 N CA C	THR B TYR B TYR B TYR B TYR B	42 43 43 43 43	77.750 76.712 75.520 75.040 75.735	41.422 43.277 44.133 44.146 44.670	75.134 77.534 77.483 76.014 75.120	1.00 36.36 1.00 31.50 1.00 30.40 1.00 30.55 1.00 29.79
55	ATOM ATOM ATOM ATOM ATOM ATOM	6058 6059 6060 6061 6062	CD2 CE1	TYR B TYR B TYR B TYR B	43 43 43 43	75.864 74.702 73.805 74.512 72.715	45.557 46.530 46.508 47.470 47.391	77.976 78.032 79.066 77.042 79.109	1.00 29.97 1.00 28.32 1.00 26.99 1.00 27.08 1.00 27.36
60	ATOM ATOM ATOM ATOM	6063 6064 6065 6066 6067	CE2 CZ OH N CA	TYR B TYR B TYR B THR B THR B	43 43 43 44	73.467 72.557 71.501 73.881 73.467	48.335 48.300 49.199 43.556 43.377	77.081 78.113 78.147 75.748 74.351	1.00 28.70 1.00 27.28 1.00 28.22 1.00 30.61 1.00 31.45
65	ATOM ATOM ATOM ATOM ATOM	6068 6069 6070 6071 6072	C O CB OG1 CG2	THR B THR B THR B THR B	44 44 44 44	72.530 72.050 72.778 71.592 73.598	44.459 45.329 42.027 42.008 40.874	73.804 74.531 74.174 74.944 74.752	1.00 31.97 1.00 32.10 1.00 31.45 1.00 32.12 1.00 33.15
70	ATOM ATOM ATOM ATOM	6073 6074 6075 6076	N CA C O	LEU B LEU B LEU B	45 45 45 45	72.258 71.322 69.951 69.219	44.387 45.317 45.080 46.016	72.503 71.886 72.518 72.820	1.00 32.35 1.00 32.17 1.00 32.45 1.00 34.45

	ATOM	6077	СВ	LEU	В	45	71.277	45.089	70.376	1.00	31.73
	ATOM	6078	ĊĞ	LEU		45	70.268	45.920	69.570		31.61
	ATOM	6079	CD1			45	70.556	47.392	69.759	1.00	
	ATOM	6080	CD2	LEU	В	45	70.220	45.528	68.036	1.00	
5	ATOM	6081	N	THR	В	46	69.577	43.835	72.715	1.00	32.08
	ATOM	6082	CA	THR	В	46	68.289	43.560	73.345		32.44
	ATOM	6083	С	THR	В	46	68.264	44.073	74.798		31.32
	ATOM	6084	0	THR		46	67.229	44.472	75.275		30.32
	MOTA	6085	CB	THR		46	67.985	42.039	73.325		32.87
10	ATOM	6086	OG1			46	67.778	41.617	71.991		33.53
	MOTA	6087	CG2			46	66.664	41.732	73.905		33.39
	ATOM	6088	N	ASP		47	69.396	44.063	75.504		30.43
	ATOM	6089	CA	ASP		47	69.383	44.642	76.843		30.27
15	ATOM	6090	C	ASP		47	69.012	46.124	76.753		29.58
15	ATOM ATOM	6091 6092	O CB	ASP ASP		47 47	68.184 70.711	46.602 44.462	77.495 77.579		28.74 30.15
	ATOM	6093	CG	ASP		47	70.711	43.013	77.958	1.00	29.26
	ATOM	6094		ASP		47	70.064	42.291	78.382	1.00	28.86
	ATOM	6095		ASP		47	72.127	42.522	77.875		29.48
20	ATOM	6096	N	TYR		48	69.570	46.824	75.786	1.00	29.34
	ATOM	6097	CA	TYR		48	69.287	48.234	75.649		29.95
	ATOM	6098	С	TYR		48	67.869	48.475	75.180		30.53
	ATOM	6099	0	TYR	В	48	67.152	49.340	75.738	1.00	29.81
	ATOM	6100	CB	TYR	В	48	70.275	48.878	74.675		30.20
25	MOTA	6101	CG	TYR		48	69.859	50.254	74.224	1.00	29.34
	ATOM	6102	CD1			48	69.649	51.273	75.144		28.33
	ATOM	6103	CD2			48	69.650	50.521	72.891	1.00	29.07
	ATOM	6104	CE1			48	69.270	52.514	74.737		27.28
20	ATOM	6105	CE2			48	69.263	51.773	72.458	1.00	27.71
30	ATOM	6106 6107	CZ	TYR		48 48	69.056 68.681	52.741 53.952	73.376 72.932		28.43
	ATOM ATOM	6108	OH N	TYR LEU		49	67.438	47.687	74.195		30.94
	ATOM	6109	CA	LEU		49	66.091	47.858	73.649		32.45
	ATOM	6110	C	LEU		49	64.983	47.561	74.640		33.72
35	ATOM	6111	ŏ	LEU		49	64.011	48.295	74.713		33.40
	ATOM	6112	ČВ	LEU		49	65.920	46.998	72.387		32.26
	ATOM	6113	CG	LEU		49	66.194	47.788	71.098		31.99
	ATOM	6114	CD1	LEU	В	49	67.040	48.975	71.308	1.00	29.89
	ATOM	6115	CD2	LEU		49	66.713	46.908	69.977		33.89
40	ATOM	6116	N	LYS		50	65.121	46.481	75.400		35.26
	MOTA	6117	CA	LYS		50	64.090	46.107	76.374		37.22
	ATOM	6118	C	LYS		50	64.293	46.640	77.806		37.29
	ATOM	6119	O	LYS		50	63.612	46.202	78.711		37.02
45	ATOM ATOM	6120 6121	CB CG	LYS LYS		50 50	64.007 63.593	44.583 43.860	76.466 75.230	1.00	38.22 40.87
43	ATOM	6122	CD	LYS		50	64.223	42.456	75.249	1.00	
	ATOM	6123	CE	LYS		50	63.689	41.520	76.384		49.69
	ATOM	6124	NZ	LYS		50	64.640	40.396	76.655		49.70
	ATOM	6125	N	ASN	_	51	65.261	47.520	78.031		38.20
50	ATOM	6126	CA	ASN		51	65.390	48.144	79.339		39.09
	ATOM	6127	C	ASN	В	51	65.606	47.121	80.454	1.00	39.31
	ATOM	6128	0	ASN	В	51	65.004	47.216	81.504		39.91
	MOTA	6129	CB	ASN		51	64.085	48.890	79.618		39.37
	MOTA	6130	CG	ASN		51	64.298	50.254	80.233		42.26
55	MOTA	6131	OD1	ASN		51	63.738	50.571	81.293		46.59
	MOTA	6132	ND2	ASN		51	65.079	51.081	79.569		42.03
	ATOM	6133	N	THR		52	66.453	46.134	80.227		39.39
	ATOM	6134	CA	THR		52	66.643	45.080	81.204		39.63
60	ATOM ATOM	6135 6136	C	THR THR		52 52	67.329 67.029	45.541 45.023	82.496 83.560		39.19 38.43
00	ATOM	6137	O CB	THR		52	67.446	43.023	80.573		39.59
	ATOM	6138	OG1	THR		52	66.824	43.570	79.348		40.44
	ATOM	6139	CG2	THR		52	67.349	42.695	81.412		40.57
	ATOM	6140	N CG2	TYR		53	68.240	46.497	82.356		38.59
65	ATOM	6141	CA	TYR		53	68.989	47.077	83.443		38.99
	ATOM	6142	C.	TYR		53	68.498	48.514	83.663		39.15
	ATOM	6143	ō	TYR		53	68.932	49.451	82.998		39.02
	MOTA	6144	CB	TYR		53	70.484	46.999	83.109		38.55
	ATOM	6145	CG	TYR		53	70.948	45.564	82.960		38.41
70	MOTA	6146	CD1	TYR	В	53	70.925	44.687	84.034	1.00	39.45

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5	ATOM ATOM ATOM ATOM ATOM	6147 6148 6149 6150	CE CE CE	E2 TYR I	B 53 B 53 B 53	71.337 71.769 71.749	45.067 43.341 43.737 42.889 41.588	83.885 81.580 82.650	1.00 40.17 1.00 39.74 1.00 39.48
	ATOM ATOM ATOM ATOM	6152 6153 6154 6155	N CA C	ARG I	54 54 3 54 3 54	67.580 66.880 67.437	48.668 49.929 50.820	84.606 84.811 85.918	1.00 39.82 1.00 41.09 1.00 39.95
10	ATOM ATOM ATOM	6156 6157 6158	CB CG CD	ARG E ARG E ARG E	54 54 54 54	67.650 65.419 64.600 63.077	50.345 49.637 49.054 48.880	85.167 84.064	1.00 42.08 1.00 48.62 1.00 54.89
15	ATOM ATOM ATOM ATOM ATOM	6159 6160 6161 6162 6163	CZ NH NH	ARG E 1 ARG E 2 ARG E	54 54 54 54	62.411 61.659 61.460 61.103	47.906 48.219 49.488 47.254	83.531 82.463 82.109 81.736	1.00 59.33 1.00 63.36 1.00 64.50 1.00 64.31
20	ATOM ATOM ATOM ATOM ATOM	6163 6164 6165 6166	CA C O	LEU E LEU E LEU E LEU E	55 55 55	67.624 68.019 66.848 65.761	52.099 53.106 53.477 53.777	85.602 86.583 87.458 86.954	1.00 38.60 1.00 38.98 1.00 38.29 1.00 37.51
25	ATOM ATOM ATOM ATOM	6168 6169 6170 6171	CG CD CD	LEU E 1 LEU B 2 LEU B	55 55 55	68.541 69.895 70.193 70.922	54.365 54.108 55.111 54.157	85.898 85.263 84.136 86.320	1.00 38.96 1.00 41.05 1.00 43.07 1.00 41.53
23	ATOM ATOM ATOM	6172 6173 6174	N CA C	LYS B LYS B LYS B LYS B	56 56 56	67.047 65.993 66.122 67.226	53.395 53.746 55.239 55.745	88.774 89.732 90.005 90.142	1.00 37.79 1.00 37.45 1.00 36.19 1.00 36.81
30	ATOM ATOM ATOM ATOM	6175 6176 6177 6178	CB CG CD CE	LYS B LYS B LYS B LYS B	56 56 56	66.093 65.489 65.304 65.245	52.962 51.564 51.064 49.527	91.048 91.056 92.507 92.650	1.00 37.81 1.00 40.35 1.00 44.36 1.00 46.29
35	ATOM ATOM ATOM ATOM	6179 6180 6181 6182	NZ N CA C	LYS B LEU B LEU B LEU B	57 57 57	65.354 64.976 64.854 64.324	57.683	94.089 90.107 90.238 91.612	1.00 43.46 1.00 34.92 1.00 34.55 1.00 32.13
40	ATOM ATOM ATOM ATOM ATOM ATOM	6183 6184 6185 6186 6187 6188		LEU B LEU B LEU B LEU B TYR B	57 57 57 57 57 58	63.927 63.815 63.956 62.694 65.175	56.808 57.886 57.325 57.519 57.973	92.336 89.209 87.791 86.874 87.144	1.00 32.19 1.00 34.23 1.00 38.69 1.00 40.17 1.00 38.67
45	ATOM ATOM ATOM ATOM	6189 6190 6191 6192	CA C O CB	TYR B TYR B TYR B TYR B	58 58 58 58	64.366 63.645 63.147 63.755 64.489	58.951 59.437 60.832 61.816 59.430	91.968 93.133 92.827 93.195 94.405	1.00 30.33 1.00 28.99 1.00 28.96 1.00 28.57 1.00 28.55
50	ATOM ATOM ATOM ATOM ATOM	6193 6194 6195 6196 6197	CG CD1 CD2 CE1 CE2	TYR B TYR B	58 58 58 58 58	63.678 63.157 63.436 62.428 62.668	59.376 60.541 58.166 60.550 58.141	95.687 96.221 96.362 97.356 97.571	1.00 26.14 1.00 26.40 1.00 25.89 1.00 25.05 1.00 24.22
55	ATOM ATOM ATOM ATOM ATOM ATOM	6198 6199 6200 6201 6202 6203	CZ OH N CA C	TYR B TYR B SER B SER B SER B SER B	58 59 59 59 59	62.169 61.443 62.014 61.351 60.397 59.401	59.359 59.503 60.891 62.127 62.561	98.037 99.176 92.154 91.819 92.896	1.00 27.02 1.00 27.44 1.00 28.77 1.00 28.72 1.00 28.49
60	ATOM ATOM ATOM ATOM	6204 6205 6206 6207	CB OG N CA	SER B SER B LEU B LEU B	59 59 60	60.541 61.360 60.662 59.803	61.897 61.917 61.214 63.723 64.224	93.153 90.537 89.608 93.479	1.00 27.25 1.00 29.06 1.00 31.54 1.00 28.81
65	ATOM ATOM ATOM ATOM ATOM	6208 6209 6210 6211 6212	C O CB CG	LEU B LEU B LEU B LEU B	60 60 60 60	59.803 59.311 59.855 60.532 61.605 62.895	64.224 65.609 66.219 64.214 65.189 64.477	94.518 94.189 93.299 95.864 96.362	1.00 29.07 1.00 30.02 1.00 29.55 1.00 28.50 1.00 29.47
70	ATOM ATOM ATOM ATOM	6213 6214 6215 6216		LEU B ARG B ARG B ARG B	60 61 61 61	61.809 58.277 57.791 57.674	64.477 66.511 66.087 67.457 68.106	96.481 95.678 94.889 94.701 96.066	1.00 32.38 1.00 28.57 1.00 30.95 1.00 32.76 1.00 31.69

	ATOM	6217	0	ARG		61	56.88				32.62
	ATOM ATOM	6218 6219	CB CG	ARG		61 61	56.43 56.30			1.00	33.00 37.71
	ATOM	6220	CD	ARG		61	54.91				43.84
5	ATOM	6221	NE	ARG		61	54.76				46.60
	ATOM	6222	CZ	ARG		61	53.63			1.00	
	MOTA	6223	NH1			61	52.52	-		1.00	
	MOTA	6224	NH2			61	53.59				49.42
10	ATOM	6225	N	TRP		62	58.48			1.00	30.71
10	MOTA MOTA	6226 6227	CA	TRP TRP		62 62	58.43 57.09			1.00	31.67
	ATOM	6228	C O	TRP		62	56.61			1.00	31.76 30.27
	ATOM	6229	СВ	TRP		62	59.55			1.00	30.92
	MOTA	6230	CG	TRP		62	60.88			1.00	31.46
15	ATOM	6231	CD1	TRP	В	62	61.89	4 70.191	96.920	1.00	29.49
	ATOM	6232	CD2			62	61.34			1.00	31.13
	ATOM	6233	NE1			62	62.96			1.00	31.80
	ATOM	6234	CE2	TRP		62	62.65			1.00	29.69
20	ATOM ATOM	6235 6236	CE3 CZ2	TRP TRP		62 62	60.78 63.41			1.00	26.50
20	ATOM	6237	CZ2	TRP		62	61.54			1.00	31.02 31.33
	ATOM	6238	CH2			62	62.84			1.00	
	ATOM	6239	N	ILE		63	56.51				32.74
	MOTA	6240	CA	ILE		63	55.20				33.71
25	ATOM	6241	С	ILE	В	63	55.15		100.103	1.00	33.06
	ATOM	6242	0	ILE		63	54.10				32.38
	ATOM	6243	CB	ILE		63	54.25			1.00	
	ATOM	6244 6245	CG1			63	53.25		98.088		36.41
30	MOTA ATOM	6245	CG2 CD1	ILE		63 63	53.74 52.96		100.673 97.611	1.00	35.85 38.12
30	ATOM	6247	N	SER	_	64	56.28		100.773	1.00	
	ATOM	6248	CA	SER		64	56.41		101.799		32.02
	ATOM	6249	C	SER		64	57.88		102.100		32.02
	ATOM	6250	0	SER	В	64	58.67	8 73.007	101.290	1.00	31.20
35	MOTA	6251	CB	SER		64	55.62		103.047		32.59
	MOTA	6252	OG	SER		64	56.13		103.603		30.59
	ATOM	6253	N	ASP	В		58.26		103.249		33.10
	ATOM ATOM	6254 6255	CA C	ASP ASP		65 65	59.67 60.24		103.598 104.207	1.00	34.48 33.71
40	ATOM	6256	0	ASP		65	61.45		104.207	1.00	
10	ATOM	6257	СВ	ASP		65	59.96		104.542	1.00	
	ATOM	6258	ĊĞ	ASP		65	59.33		105.936		39.93
	ATOM	6259		ASP		65	58.31	7 74.376	106.106	1.00	41.80
	ATOM	6260	OD2	ASP	В	65	59.77		106.938	1.00	46.16
4 5	ATOM	6261	N	HIS		66	59.39		104.520		33.76
	ATOM	6262	CA	HIS		66	59.86		105.209		34.50
	ATOM ATOM	6263 6264	C	HIS HIS		66 66	59.22 59.44		104.805 105.458		33.72 33.16
	ATOM	6265	O CB	HIS		66	59.71		105.438		35.88
50	ATOM	6266	CG	HIS		66	58.29		107.202		38.04
	ATOM	6267		HIS		66	57.77		107.963		45.25
	MOTA	6268	CD2	HIS	В	66	57.31		107.098	1.00	43.06
	ATOM	6269		HIS		66	56.51		108.264		46.62
	ATOM	6270		HIS		66	56.20		107.751		46.13
55	ATOM	6271	N	GLU		67	58.43		103.730		32.69
	ATOM ATOM	6272 6273	CA C	GLU GLU		67 67	57.72 57.65		103.271 101.761		33.17 31.79
	ATOM	6274	Ö	GLU		67	57.59		101.701		31.79
	ATOM	6275	СВ	GLU		67	56.29		103.791		33.48
60	ATOM	6276	CG	GLU		67	56.11		105.296		37.72
	ATOM	6277	CD	GLU		67	54.65		105.672		42.22
	MOTA	6278	OE1	GLU		67	54.16		105.378		48.76
	ATOM	6279	OE2	GLU		67	53.99		106.228		42.33
75	ATOM	6280	N	TYR		68	57.63		101.256		30.97
65	ATOM ATOM	6281 6282	CA	TYR		68 68	57.509 56.59		99.825 99.528		29.71
	ATOM	6282	C O	TYR TYR		68	56.32		100.413		29.93 29.08
	ATOM	6284	СВ	TYR		68	58.87		99.185		29.52
	ATOM	6285	ĊĠ	TYR		68	59.66		99.671		28.39
70	ATOM	6286	CD1	TYR		68	59.36		99.220		22.82

		ATOM ATOM	6287 6288		2 TYR 1 TYR		68 68		0.730			100.587		0 28.35
		ATOM	6289				68		50.087 51.479			99.624 101.005		0 23.16 0 29.42
		ATOM	6290		TYR		68		1.137			100.526		0 29.42
	5	ATOM	6291		TYR		68		1.857	61.7	41	100.912	1.00	26.61
		ATOM ATOM	6292 6293		LEU		69		6.127			98.281	1.00	29.92
		ATOM	6294		LEU LEU		69 69		5.358 6.188			97.786 96.978	1.00	30.28
		ATOM	6295	_	LEU		69		7.070			96.218		30.18 30.00
	10	ATOM	6296	CB	LEU	В (69		4.194			96.895		30.22
		ATOM	6297	CG	LEU		59		3.193			97.530	1.00	30.36
		ATOM ATOM	6298 6299		LEU LEU		59 59		2.388 2.338			96.405		34.17
		ATOM	6300	N N	TYR		70		5.833			98.468 97.085		31.47 31.67
	15	ATOM	6301	CA	TYR	в 7	70		6.553			96.424		33.09
		ATOM	6302	C	TYR		70		5.561			96.272	1.00	34.91
		ATOM ATOM	6303 6304	O CB	TYR TYR		70 70		4.762 7.730			97.179		35.21
		ATOM	6305	CG	TYR		70		8.487			97.296 96.681		33.20 34.09
	20	ATOM	6306	CD1	. TYR	B 7	70		9.342			95.613		34.32
		ATOM	6307	CD2			70		8.333	58.08		97.159	1.00	36.48
		ATOM ATOM	6308 6309	CE1 CE2			70 70	_	0.027 9.017	58.53		95.043		35.68
		ATOM	6310	CZ	TYR		0		9.859	57.03 57.25		96.607 95.554		38.59 38.10
	25	MOTA	6311	OH	TYR		'Õ		0.530	56.17		95.042		38.44
		MOTA	6312	N	LYS		1		5.580	59.21		95.132	1.00	37.42
		ATOM ATOM	6313 6314	CA C	LYS LYS		'1 '1		4.665	58.13		94.922		39.82
		ATOM	6315	Ö	LYS .		1		5.395 6.472	56.78 56.57		95.087 94.523		41.07 40.84
	30	ATOM	6316	CB	LYS		1		3.902	58.29		93.598		40.28
		ATOM	6317	CG	LYS		1		4.600	57.90		92.345	1.00	43.25
		ATOM ATOM	6318 6319	CD CE	LYS :		1 1		3.531 3.486	57.75 58.96		91.197		48.13
		ATOM	6320	NZ	LYS		1		3.741	60.29		90.240 90.932		48.89 47.42
	35	ATOM	6321	N	GLN :	в 7	2		4.823	55.92		95.926		42.40
		ATOM	6322	CA	GLN I		2		5.399	54.62		96.244	1.00	44.10
		ATOM ATOM	6323 6324	С О	GLN I		2 2		4.321 3.281	53.57 53.65		96.095		45.27
		ATOM	6325	СВ	GLN I				5.910	54.63		96.762 97.691		44.58 44.50
	40	ATOM	6326	CG	GLN I			56	5.800	53.46		98.088		44.48
		ATOM ATOM	6327 6328	CD	GLN I				7.329	53.63		99.503		44.96
		ATOM	6329		GLN I				5.615 3.576	53.37		00.474 99.621		43.70 45.53
		ATOM	6330	N	GLU I				1.569	52.60		95.211		47.20
•	45	ATOM	6331	CA	GLU I				3.630	51.50	5	94.957	1.00	48.73
		ATOM ATOM	6332 6333	C O	GLU I			52	2.286	52.15		94.671		48.68
		ATOM	6334	CB	GLU E				.254	51.78 50.54		95.215 96.158		48.41 49.31
		ATOM	_	CG	GLU E				.947	50.02		96.582		51.35
	50	ATOM	6336	CD	GLU E			54	.871	48.83	3	97.530	1.00	54.65
		ATOM ATOM	6337 6338	OE1	GLU E				.276	47.78		97.142		55.54
		ATOM	6339	N	GLU E				.408	48.94 53.07		98.663 93.718		54.55 49.04
		ATOM	6340	CA	ASN E				.376	54.10		93.416	1.00	49.04
5	55	ATOM	6341	C	ASN E			50	.382	54.60	3	94.488	1.00	47.27
		ATOM ATOM	6342 6343	0	ASN E				.229	54.93		94.228		46.85
		ATOM	6344	CB CG	ASN E				.854	54.00 54.74		91.978 91.011		50.33
		ATOM	6345		ASN E				.026	54.63		91.147		53.96 59.25
6	60	ATOM	6346	ND2	ASN E	3 74		51	.243	55.54	1	90.102		58.66
		ATOM	6347	N	ASN E			50	.912	54.71		95.701		45.27
		ATOM ATOM	6348 6349	CA C	ASN E			50 50	.285 .971	55.49		96.736		43.89
		ATOM	6350	Ö	ASN B				.152	56.866 56.948		96.625 96.357		42.53 42.77
6	55	MOTA	6351	СВ	ASN B	75	5	50	.559	54.93	4 !	98.133		43.56
		ATOM	6352	CG	ASN B				.860	53.600	0 !	98.387	1.00	42.32
		ATOM ATOM	6353 6354		ASN B				.634 .651	53.518 52.560		98.429		38.62
		ATOM	6355	N	ILE B				.231	57.94		98.593 96.807		43.37
7	0	ATOM	6356	CA	ILE B				.842	59.23		96.857		38.95

5	ATOM ATOM ATOM ATOM ATOM ATOM	6357 6358 6359 6360 6361 6362	C O CB CG1 CG2 CD1	ILE B	76 76 76 76 76 76	51.150 50.255 49.910 49.892 50.395 49.030	59.520 59.693 60.272 60.098 61.665 61.130	98.314 99.109 96.247 94.722 96.574 94.000	1.00 1.00 1.00 1.00	36.65 34.71 39.60 40.79 40.25 43.78
10	ATOM ATOM ATOM	6363 6364 6365	N CA C	LEU B LEU B LEU B	77 77 77	52.433 52.846 53.402	59.560 59.775 61.163	98.653 100.024 100.234	1.00 1.00 1.00	34.92 33.64 33.19
10	ATOM ATOM ATOM ATOM	6366 6367 6368 6369	O CB CG CD1		77 77 77 77	53.918 53.966 53.902 55.169	57.317 56.615	99.277 100.384 100.033 100.550	1.00 1.00	32.58 33.67 34.31 34.52
15	ATOM ATOM ATOM ATOM	6370 6371 6372 6373	CD2 N CA C	LEU B VAL B VAL B	77 78 78 78	52.668 53.250 54.007 55.108	61.669 62.830 62.367	100.612 101.463 101.890 102.840	1.00 1.00 1.00	35.27 32.23 32.17 31.20
20	ATOM ATOM ATOM ATOM	6374 6375 6376 6377	O CB CG1 CG2	VAL B	78 78 78 78	54.875 53.184 54.002 51.968	63.855 65.131 64.185	103.751 102.689 102.964 101.960	1.00 1.00 1.00	30.88 33.20 32.36 35.58
25	ATOM ATOM ATOM ATOM	6378 6379 6380 6381	N CA C O	PHE B PHE B PHE B	79 79 79 79	56.279 57.414 57.793 57.673	62.708 63.902 65.025	102.678 103.545 104.376 103.911	1.00 1.00 1.00	30.94 30.29 30.36 30.80
	ATOM ATOM ATOM ATOM	6382 6383 6384 6385	CB CG CD1 CD2	PHE B PHE B PHE B	79 79 79 79	58.618 58.592 57.732 59.397	60.885 60.454	102.715 102.308 101.311 102.960		29.20
30	ATOM ATOM ATOM ATOM	6386 6387 6388 6389	CE1 CE2 CZ N	PHE B PHE B PHE B ASN B	79 79 79 80	57.723 59.382 58.554 58.255	58.639 58.211	100.964 102.614 101.632 105.598		30.10 25.52 25.12 29.03
35	ATOM ATOM ATOM ATOM	6390 6391 6392 6393	CA C O CB	ASN B ASN B ASN B	80 80 80 80	58.741 60.256 60.900 58.296	64.705 63.712	106.465 106.318 106.556 107.898	1.00 1.00	29.19 29.44 30.11 28.74
40	ATOM ATOM ATOM ATOM ATOM	6394 6395 6396 6397 6398	CG	ASN B ASN B ASN B ALA B ALA B	80 80 80 81 81	58.948 60.147 58.157 60.821 62.222	65.268 66.173 65.817	108.888 109.094 109.536 105.904 105.590	1.00 1.00 1.00	29.09 29.35 25.89 29.51 30.69
45	ATOM ATOM ATOM ATOM	6399 6400 6401 6402	С О СВ N	ALA B ALA B ALA B GLU B	81 81 81 82	63.150 64.079 62.563 62.895	65.623 64.840 67.148 66.310	106.792 106.699 104.873 107.895	1.00 1.00 1.00 1.00	30.80 30.60 29.54 31.58
50	MOTA MOTA ATOM ATOM	6403 6404 6405 6406	CA C O CB	GLU B GLU B GLU B	82 82 82 82	63.749 63.857 64.960 63.221	64.795 64.303 67.083	109.744 110.215	1.00 1.00 1.00	32.74 32.27 32.51 33.43
	ATOM ATOM ATOM ATOM	6407 6408 6409 6410	CG CD OE1 OE2	GLU B	82 82 82 82	64.199 65.576 65.677 66.566	68.473 67.193	110.968 110.041 111.557	1.00 1.00 1.00	36.43 40.84 44.66 43.16
55	MOTA MOTA MOTA	6411 6412 6413 6414	N CA C O	TYR B TYR B TYR B TYR B	83 83 83	62.717 62.684 62.452 62.676	62.779 61.596 60.488	109.367 109.780	1.00 1.00 1.00	30.92 30.84 30.26 29.50
60	ATOM ATOM ATOM ATOM	6415 6416 6417 6418	CD2		83 83 83	61.628 61.864 62.976 61.007	62.731 63.793 63.736 64.870	112.364 113.187 112.488	1.00 1.00 1.00	29.67 30.76 32.90 29.61
65	ATOM ATOM ATOM ATOM	6419 6420 6421 6422	CE2 CZ OH	TYR B TYR B	83 83 83	63.228 61.244 62.379 62.650	64.728 65.857 65.786 66.746	113.414 114.221 115.181	1.00 1.00 1.00	32.38 32.14 34.48 40.18
70	ATOM ATOM ATOM ATOM	6423 6424 6425 6426	N CA C O	GLY B GLY B GLY B	84 84 84	61.971 61.819 60.520 60.257	61.788 60.641 59.863 58.998	107.265 107.382	1.00 1.00	30.54 30.76 30.75 31.47

	ATOM	6427	N	ASN 1	3 85	E0 (01 (0 120 100 205 1 00 01 01
	ATOM	6428				59.691 60.138 108.387 1.00 31.23 58.399 59.446 108.443 1.00 31.63
	ATOM	6429	C	ASN I	85	58.399 59.446 108.443 1.00 31.69 57.477 59.915 107.279 1.00 32.1
5	ATOM	6430		ASN I		57.537 61.063 106.852 1.00 30.53
3	ATOM ATOM	6431 6432				57.699 59.607 109.803 1.00 30.47
	ATOM	6433		1 ASN E		57.315 61.007 110.089 1.00 31.43 58.191 61.876 110.191 1.00 33.75
	ATOM	6434				56.000 61.269 110.198 1.00 33.75
• •	ATOM	6435		SER E		56.628 59.017 106.810 1.00 33.47
10		6436	_	SER E		55.761 59.280 105.674 1.00 35.12
	ATOM ATOM	6437 6438		SER E		54.369 58.849 105.986 1.00 36.58 54.146 58.032 106.877 1.00 36.18
	ATOM	6439		SER E		54.146 58.032 106.877 1.00 36.15 56.200 58.460 104.490 1.00 35.25
	MOTA	6440	OG	SER E		56.483 57.165 104.932 1.00 37.10
15		6441	N	SER E		53.430 59.419 105.242 1.00 37.64
	ATOM ATOM	6442 6443	CA C	SER E		52.028 59.089 105.364 1.00 38.75
	ATOM	6444	Ö	SER E		51.394 59.084 103.977 1.00 39.14 51.930 59.651 103.026 1.00 39.55
	ATOM	6445	ČВ	SER B		51.930 59.651 103.026 1.00 39.55 51.290 60.079 106.264 1.00 39.10
20	MOTA	6446	OG	SER B		51.755 59.996 107.591 1.00 40.45
	ATOM	6447	N	VAL B		• 50.239 58.434 103.889 1.00 39.63
	MOTA MOTA	6448 6449	CA C	VAL B		49.509 58.296 102.643 1.00 40.87
	ATOM	6450	Ö	VAL B		48.643 59.539 102.386 1.00 41.23 47.661 59.782 103.086 1.00 40.79
25	ATOM	6451	СВ	VAL B	88	48.631 57.004 102.636 1.00 41.06
	ATOM	6452		VAL B		48.060 56.712 104.036 1.00 43.96
	ATOM ATOM	6453 6454	CG2 N	VAL B	88	47.525 57.135 101.592 1.00 40.56
	ATOM	6455	CA	PHE B	89 89	49.022 60.312 101.378 1.00 42.05 48.214 61.446 100.964 1.00 43.87
30	ATOM	6456	C	PHE B	89	48.214 61.446 100.964 1.00 43.87 46.989 61.027 100.163 1.00 44.21
	ATOM	6457	0	PHE B	89	45.917 61.555 100.345 1.00 43.68
	ATOM ATOM	6458	CB	PHE B	89	49.002 62.442 100.126 1.00 44.25
	ATOM	6459 6460	CG CD1	PHE B	89 89	48.279 63.735 99.959 1.00 46.62 48.319 64.690 100.960 1.00 49 83
35	ATOM	6461		PHE B	89	48.319 64.690 100.960 1.00 49.83 47.494 63.967 98.849 1.00 48.66
	MOTA	6462	CE1	PHE B	89	47.617 65.874 100.831 1.00 50.73
	ATOM	6463		PHE B	89	46.785 65.136 98.725 1.00 49.25
	ATOM ATOM	6464 6465	CZ N	PHE B LEU B	89 90	46.848 66.088 99.719 1.00 50.32
40	ATOM	6466	CA	LEU B	90	47.173 60.072 99.268 1.00 45.65 46.098 59.577 98.434 1.00 47.32
	MOTA	6467	C	LEU B	90	46.329 58.093 98.306 1.00 48.48
	ATOM	6468	0	LEU B	90	47.341 57.680 97.752 1.00 47.19
	ATOM ATOM	6469 6470	CB CG	LEU B	90	46.192 60.220 97.050 1.00 47.51
45	ATOM	6471	CD1		90 90	44.961 60.573 96.237 1.00 49.43 45.201 60.128 94.783 1.00 50.89
	ATOM	6472		LEU B	90	43.731 59.945 96.784 1.00 50.36
	ATOM	6473	N	GLU B	91	45.387 57.302 98.804 1.00 50.77
	ATOM ATOM	647 4 6475	CA		91	45.523 55.845 98.815 1.00 53.33
50	ATOM	6476	C O	GLU B	91 9 1	45.681 55.245 97.410 1.00 54.61 44.958 55.617 96.503 1.00 53.67
	ATOM	6477	ČВ	GLU B	91	44.958 55.617 96.503 1.00 53.67 44.312 55.185 99.494 1.00 53.90
	ATOM	6478	CG	GLU B	91	43.496 56.067 100.445 1.00 56.83
	ATOM ATOM	6479	CD OD1	GLU B	91	42.375 56.850 99.752 1.00 60.34
55	ATOM	6480 6481		GLU B	91 91	42.639 57.978 99.252 1.00 59.61 41.226 56.325 99.707 1.00 62.58
	ATOM	6482	N	ASN B	92	41.226 56.325 99.707 1.00 62.58 46.617 54.305 97.244 1.00 56.76
	ATOM	6483	CA	ASN B	92	46.790 53.626 95.957 1.00 58.76
	ATOM	6484	C	ASN B	92	45.440 53.196 95.373 1.00 60.58
60	ATOM ATOM	6485	O	ASN B	92	45.181 53.331 94.167 1.00 60.40
00	ATOM	6486 6487		ASN B ASN B	92 92	47.755 52.412 96.063 1.00 58.98 47.259 51.311 97.022 1.00 59.52
	ATOM	6488	OD1	ASN B	92	47.259 51.311 97.022 1.00 59.52 46.362 51.542 97.840 1.00 60.59
	ATOM	6489	ND2	ASN B	92	47.817 50.094 96.897 1.00 61.81
C F	ATOM	6490	N	SER B	93	44.580 52.720 96.264 1.00 62.60
65	ATOM ATOM	6491 6492	CA C	SER B SER B	93 93	43.268 52.168 95.922 1.00 64.67
	ATOM	6493		SER B	93	42.282 53.169 95.329 1.00 65.69 41.597 52.858 94.344 1.00 66.09
	ATOM	6494		SER B	93	41.597 52.858 94.344 1.00 66.09 42.659 51.570 97.187 1.00 64.77
70	ATOM	6495		SER B	93	43.699 51.255 98.109 1.00 66.81
70	ATOM	6496	N	THR B	94	42.182 54.349 95.943 1.00 66.89

		_								
	ATOM	6497	CA	THR		94	41.285	55.377	95.440	1.00 67.90
	ATOM	6498	C	THR		94	41.516		93.950	1.00 68.67
	MOTA	6499	0	THR		94	42.652	55.387	93.481	1.00 68.63
5	ATOM ATOM	6500 6501	CB OG1	THR THR		94 94	41.571 42.354	56.749 56.609	96.064 97.254	1.00 68.14 1.00 67.83
,	ATOM	6502	CG2			94	40.274	57.410	96.532	1.00 67.83
	ATOM	6503	N CG2	PHE		95	40.430	55.583	93.207	1.00 69.89
	ATOM	6504	CA	PHE		95	40.497	55.602	91.754	1.00 70.65
	ATOM	6505	C	PHE		95	40.944	54.252	91.233	1.00 70.03
10	ATOM	6506	ŏ	PHE		95	42.029	54.099	90.678	1.00 71.18
	ATOM	6507	ČВ		В	95	41.392	56.735	91.256	1.00 70.73
	ATOM	6508	CG	PHE		95	41.049	58.049	91.865	1.00 70.42
	ATOM	6509	CD1	PHE		95	39.734	58.469	91.910	1.00 70.08
	ATOM	6510	CD2	PHE	В	95	42.025	58.840	92.435	1.00 70.08
15	ATOM	6511	CE1	PHE	В	95	39.403	59.654	92.493	1.00 69.12
	MOTA	6512		PHE		95	41.691	60.030	93.014	1.00 70.02
	ATOM	6513	CZ	PHE		95	40.376	60.433	93.041	1.00 69.12
	ATOM	6514	N	ASP		96	40.085	53.276	91.501	1.00 71.95
	ATOM	6515	CA	ASP		96	40.174	51.930	90.968	1.00 72.26
20	ATOM	6516	C	ASP		96	38.920	51.861	90.104	1.00 72.48
	ATOM	6517	0	ASP		96	38.931	51.431	88.940	1.00 72.15
	MOTA	6518	CB	ASP		96	40.089	50.885	92.094	1.00 72.41
	ATOM	6519 6520	CG	ASP		96	41.452	50.303	92.491	1.00 72.76
25	ATOM ATOM	6521	OD1 OD2			96 96	42.461 41.606	50.610 49.509	91.830 93.450	1.00 74.22 1.00 71.03
23	ATOM	6522	N N	GLU		97	37.831	52.337	90.701	1.00 71.03 1.00 72.66
	ATOM	6523	CA	GLU		97	36.521	52.362	90.067	1.00 72.60
	ATOM	6524	C	GLU		97	36.261	53.683	89.321	1.00 72.00
	ATOM	6525	ŏ	GLU		97	35.142	53.933	88.872	1.00 71.85
30	ATOM	6526	ČВ	GLU		97	35.486	52.159	91.167	1.00 73.02
	ATOM	6527	CG	GLU		97	34.042	52.011	90.723	1.00 74.39
	ATOM	6528	CD	GLU		97	33.130	51.759	91.910	1.00 76.22
	ATOM	6529	OE1	GLU	В	97	33.579	52.004	93.059	1.00 76.78
	ATOM	6530	OE2	GLU	В	97	31.979	51.313	91.696	1.00 76.84
35	ATOM	6531	N		В	98	37.294	54.518	89.175	1.00 70.65
	ATOM	6532	CA		В	98	37.139	55.807	88.505	1.00 69.57
	ATOM	6533	C		В	98	36.692	55.642	87.051	1.00 68.08
	ATOM	6534	0		В	98	35.986	56.486	86.522	1.00 68.19
40	ATOM	6535	CB		В	98	38.429	56.624	88.577	1.00 69.94
40	ATOM	6536 6537	CG		В	98 98	38.381	57.894 58.887	87.772	1.00 70.49 1.00 70.34
	ATOM ATOM	6538	CD1 CD2		B B	98	37.458 39.246	58.088	88.073 86.701	1.00 70.34 1.00 71.59
	ATOM	6539	CE1		В	98	37.411	60.063	87.333	1.00 71.33
	ATOM	6540	CE2		В	98	39.201	59.267	85.947	1.00 70.03
45	ATOM	6541	CZ		В	98	38.281	60.255	86.270	1.00 71.03
	ATOM	6542	N		В	99	37.099	54.564	86.398	1.00 66.41
	MOTA	6543	CA	GLY	В	99	36.599	54.293	85.060	1.00 65.26
	MOTA	6544	С	GLY	В	99	37.471	54.761	83.913	1.00 63.94
	ATOM	6545	0	GLY	В	99	37.077	54.635	82.743	1.00 63.67
50	ATOM	6546	N	HIS		100	38.636	55.311	84.252	1.00 62.08
	ATOM	6547	CA	HIS		100	39.618	55.740	83.269	1.00 60.54
	ATOM	6548	C	HIS		100	41.006	55.611	83.858	1.00 58.93
	ATOM	6549	0	HIS		100	41.216	55.858	85.042	1.00 58.09
	ATOM	6550	CB	HIS		100	39.495	57.227	82.924	1.00 60.44
55	ATOM	6551	CG	HIS		100	38.131	57.681	82.520	1.00 60.43
	ATOM ATOM	6552 6553		HIS			37.367	58.516	83.309	1.00 61.86
	ATOM	6554		HIS HIS			37.435 36.236	57.506 58.795	81.373	1.00 61.34
	ATOM	6555		HIS			36.252	58.195	82.682 81.505	1.00 61.63 1.00 60.88
60	ATOM	6556	NEZ N	SER			41.968	55.264	83.019	1.00 57.46
00	ATOM	6557	CA	SER			43.352	55.333	83.427	1.00 56.47
	ATOM	6558	CA	SER			43.620	56.813	83.736	1.00 55.22
	ATOM	6559	ŏ	SER			43.280	57.678	82.930	1.00 55.25
	ATOM	6560	ČВ	SER			44.261	54.834	82.300	1.00 56.82
65	ATOM	6561	OG	SER			45.485	55.565	82.254	1.00 57.96
	ATOM	6562	N	ILE			44.170	57.103	84.912	1.00 53.65
	ATOM	6563	CA	ILE			44.558	58.455	85.274	1.00 52.71
	ATOM	6564	C	ILE		102	46.024	58.646	84.939	1.00 51.90
	ATOM	6565	Ō	ILE	В	102	46.891	57.906	85.408	1.00 51.45
70	ATOM	6566	CB	ILE		102	44.352	58.732	86.761	1.00 52.96

	ATOM	6567	CG	1 IL	E F	102	42.88	89	59.04	0 87.04	Ω 1 1	10 E2 EC
	ATOM	6568				102	45.21		59.93			0 53.56
	ATOM	6569	CD:			102	42.54		58.86			
_	ATOM	6570				103	46.30		59.68			0 50.68
5		6571		AS	N B	103	47.63		59.88			0 50.00
	ATOM	6572	_			103	48.56	59	60.72			0 49.33
	ATOM	6573	-			103	49.77	76	60.54			0 48.89
	ATOM	6574				103	47.44		60.49		1.0	0 50.12
10	ATOM	6575				103	48.72		60.93		5 1.0	0 50.68
10		6576				103	49.18		62.04			0 52.56
	ATOM	6577				103	49.27	_	60.10			0 48.56
	ATOM ATOM	6578 6579	N			104	48.01		61.62			0 48.67
	ATOM	6580	CA			104	48.84		62.48			0 48.99
15	ATOM	6581	C O			104 104	47.92		63.15			0 48.52
15	ATOM	6582	СВ			104	46.72		62.91			0 48.70
	ATOM	6583	CG			104	49.59		63.51			0 49.21
	ATOM	6584				104	50.83		64.11			
	ATOM	6585				104	50.88 51.80		64.22			0 57.49
20	ATOM	6586	N	TY	R	105	48.47		64.55 63.99			0 51.76
	ATOM	6587	CA			105	47.66		64.58			0 48.07
	ATOM	6588	C			105	48.36		65.83			0 48.29 0 47.82
	ATOM	6589	0			105	49.55		66.008			0 47.82
	MOTA	6590	CB			105	47.50		63.623			0 48.41
25	ATOM	6591	CG			105	48.80		63.41			0 50.88
	MOTA	6592	CD1	TYP	В	105	49.28	5	64.366			53.35
	ATOM	6593	CD2	TYR	В	105	49.57	1	62.279			
	ATOM	6594	CE1			105	50.48	4	64.199		1.00	54.72
20	ATOM	6595	CE2	TYR		105	50.78		62.100	91.410		54.12
30		6596	CZ			105	51.22		63.071		1.00	54.90
	ATOM ATOM	6597	ОН	TYR		105	52.43		62.932			56.72
	ATOM	6598 6599	N			106	47.607		66.712			47.41
	ATOM	6600	CA C	SER		106	48.154		67.975			47.19
35	ATOM	6601	Ö	SER SER		106 106	47.355		68.466			47.24
	ATOM	6602	СВ			106	46.183 48.134		68,832		1.00	46.40
	ATOM	6603	OG	SER		106	48.134		69.020 70.278			47.09
	ATOM	6604	N			107	48.030		68.507		1.00	
	ATOM	6605	CA			107	47.364		68.782			47.54 47.97
40	ATOM	6606	C	ILE			47.408		70.258			47.97
	ATOM	6607	0	ILE			48.403		70.897			46.88
	MOTA	6608	CB	ILE	В	107	48.023		67.952			48.46
	ATOM	6609	CG1	ILE			48.132	2	66.494			50.38
45	ATOM	6610	CG2	ILE			47.221		68.028	96.586		48.95
45	ATOM	6611	CD1				48.792		65.516	95.824		51.53
	MOTA	6612	N	SER			46.280		70.797			46.98
	ATOM	6613	CA	SER			46.165	5	72.198	95.182	1.00	47.44
	ATOM ATOM	6614	C	SER			47.139		72.506	96.299	1.00	47.37
50	ATOM	6615 6616	O	SER			47.360		71.655	97.148		47.37
30	ATOM	6617	CB OG	SER			44.750		72.479			47.48
	MOTA	6618		SER PRO			43.908		72.555	94.511	1.00	50.87
	ATOM	6619		PRO			47.680 48.726		73.714	96.314		47.60
	ATOM	6620		PRO			48.726		74.098	97.270		48.07
55	ATOM	6621	Ö	PRO			48.884		74.084 73.537	98.701		48.47
	ATOM	6622		PRO			49.067			99.582		48.42
	ATOM	6623		PRO			48.258		75.550 75.909	96.896 95.689		48.14
	ATOM	6624		PRO			47.293		74.812	95.418		48.80
	ATOM	6625		ASP			47.118		74.732	98.915		48.07
60	ATOM	6626		ASP			46.524		74.837	100.222		48.72 48.24
	MOTA	6627		ASP			45.494		73.728	100.222		48.24 48.77
	MOTA	6628		ASP			44.331		73.942	99.609		48.77
	ATOM	6629	CB .	ASP	В 3	110	46.040		76.281	100.413		49.87
	ATOM	6630		ASP			47.234		77.315	100.391		47.85
65	ATOM	6631	OD1	ASP	В :	110	48.376			100.255		41.05
	ATOM	6632	OD2				47.150		78.556	100.515		45.53
	ATOM	6633		GLY			46.028		72.549	100.427		48.67
	ATOM	6634		GLY			45.611		71.174	100.106		47.96
70	ATOM	6635		GLY			44.234		70.538	100.027		47.65
70	ATOM	6636	0 (GLY	B 1	11	44.157		69.318	100.186		48.21

	ATOM ATOM	6637 6638	N CA	GLN E		43.191 41.828	71.280 70.757	99.681 99.688		46.73 46.55
	ATOM	6639	C	GLN E		41.368	69.958	98.453		45.92
	ATOM	6640	Ō	GLN B	112	40.404	69.189	98.507		45.81
5	ATOM	6641	СВ	GLN B		40.891	71.939	99.910		47.23
	ATOM	6642	CG	GLN B		41.335	72.836 73.776	101.085	1.00	48.40 50.36
	ATOM ATOM	6643 6644	CD OE1			40.268 39.258	73.776	101.321		51.07
	ATOM	6645	NE2			40.464		102.671	1.00	52.21
10	ATOM	6646	N	PHE B		42.057	70.122	97.334	1.00	45.08
	MOTA	6647	CA	PHE B		41.642	69.458	96.113		43.92
	ATOM	6648	C	PHE B		42.805	68.847	95.343		42.79
	ATOM ATOM	6649 6650	O CB	PHE B		43.958 40.929	69.219 70.466	95.512 95.214	1.00	42.89 43.63
15	ATOM	6651	CG	PHE B		39.750	71.099	95.848		42.05
	ATOM	6652	CD1			38.488	70.569	95.677		42.72
	MOTA	6653	CD2			39.889	72.226	96.606	1.00	39.78
	MOTA	6654	CE1			37.383	71.177	96.261		42.10
20	ATOM	6655	CE2	PHE B		38.789 37.554	72.834 72.322	97.196 97.031	1.00	40.25 41.31
20	ATOM ATOM	6656 6657	CZ N	ILE B		42.487	67.880	94.505		42.17
	ATOM	6658	CA	ILE B		43.473	67.356	93.598		41.68
	ATOM	6659	C	ILE B		42.892	67.268	92.197		40.71
	ATOM	6660	О	ILE B		41.741	66.874	92.020		40.61
25	ATOM	6661	CB	ILE B		43.966	65.991	94.062		41.42
	ATOM ATOM	6662 6663	CG1 CG2			45.153 42.860	65.574 64.986	93.200 93.970		41.62 41.11
	ATOM	6664	CD1			45.635	64.163	93.416		42.89
	ATOM	6665	N	LEU B		43.715	67.599	91.201		39.94
30	ATOM	6666	CA	LEU B		43.320	67.535	89.789		39.10
	ATOM	6667	C	LEU B		43.642	66.161	89.210		38.76
	ATOM ATOM	6668 6669	O CB	LEU B		44.777 44.130	65.737 68.536	89.259 89.002		38.30 39.65
	ATOM	6670	CG	LEU B		43.616	69.790	88.299		40.09
35	ATOM	6671		LEU B		44.778	70.170	87.397		40.91
	MOTA	6672	CD2	LEU B		42.343	69.622	87.504	1.00	38.88
	ATOM	6673	N	LEU B		42.671	65.453	88.657		38.21
	MOTA MOTA	6674 6675	CA C	LEU B		42.982 42.968	64.185 64.422	88.024 86.527		38.17 37.63
40	ATOM	6676	Ö	LEU B		41.992	64.913	85.989		37.08
	ATOM	6677	ČВ	LEU B		41.974	63.094	88.383		38.64
	ATOM	6678	CG	LEU B		41.649	62.939	89.858		39.18
	ATOM	6679		LEU B	116	40.900	61.664	90.069		41.25
45	ATOM ATOM	6680 6681	CD2	LEU B	116 117	42.905 44.063	62.919 64.061	90.652 85.870		39.01 37.51
43	ATOM	6682	N CA	GLU B	117	44.234	64.281	84.444		36.48
	ATOM	6683	C	GLU B		44.052	62.967	83.754		36.12
	ATOM	6684	0	GLU B	117	44.751	61.994	84.054	1.00	38.07
	ATOM	6685	СВ	GLU B		45.649	64.823	84.205		36.68
50	ATOM	6686	CG	GLU B		45.949 47.387	65.272 65.728	82.781 82.593		35.93 35.27
	ATOM ATOM	6687 6688	CD OE1	GLU B		48.193	64.901	82.173		37.75
	ATOM	6689	OE2	GLU B		47.718	66.905	82.825		36.09
	MOTA	6690	N	TYR B		43.138	62.902	82.817	1.00	34.75
55	MOTA	6691	CA	TYR B		42.914	61.657	82.116		34.56
	ATOM	6692	C	TYR B		42.636	61.937	80.633 80.232		34.00
	ATOM ATOM	6693 6694	O CB	TYR B		42.570 41.797	63.108 60.859	82.818		33.30 34.86
	ATOM	6695	CG	TYR B		40.404	61.439	82.742		35.02
60	MOTA	6696	CD1	TYR B		39.990	62.450	83.598		39.23
	MOTA	6697	CD2	TYR B	118	39.500	60.948	81.844		38.13
	ATOM	6698	CE1	TYR B		38.677	62.981	83.529		38.18
	ATOM	6699	CE2	TYR B		38.209	61.457	81.753		40.19
65	ATOM ATOM	6700 6701	CZ OH	TYR B		37.810 36.538	62.477 62.959	82.594 82.462		40.62
03	ATOM	6702	N	ASN B		42.518	60.876	79.834		34.57
	ATOM	6703	CA	ASN B		42.391	60.976	78.377		35.21
	MOTA	6704	C	ASN B		43.487	61.898	77.769		34.89
70	ATOM	6705	0	ASN B		43.218	62.738	76.925		34.73
70	ATOM	6706	CB	ASN B	119	41.029	61.548	77.987	I.00	35.70

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ATOM
               6707
                      CG
                           ASN B 119
                                             39.910
                                                                78.017
                                                      60.521
                                                                         1.00 38.47
       ATOM
               6708
                      OD1 ASN B 119
                                             40.140
                                                      59.326
                                                                77.869
                                                                         1.00
                                                                               40.47
       ATOM
               6709
                      ND2
                          ASN B 119
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                                                      61.004
                                                                78.174
                                                                         1.00
                                                                               38.75
       ATOM
                                             44.705
45.789
               6710
                               B 120
                      N
                           TYR
                                                      61.798
                                                               78.255
                                                                         1.00
                                                                               34.18
               6711
       ATOM
                      CA
                           TYR B 120
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62.232
                                                               77.705
                                                                         1.00
                                                                               33.43
       ATOM
               6712
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                                             46.053
                           TYR B 120
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                                                                         1.00
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               6713
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                           TYR B 120
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                                                      61.059
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                                                                               32.29
       ATOM
               6714
                      CB
                           TYR
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                               В
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                                                      62.344
                                                               78.550
                                                                               33.95
                                                                         1.00
               6715
       ATOM
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77.019
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               6716
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                          TYR B 120
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                                                                               37.16
       ATOM
               6717
                      CD2
                          TYR B 120
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                                                      63.814
                                                               78.349
                                                                         1.00
                                                                               37.19
       MOTA
               6718
                      CE1
                          TYR
                               B 120
                                            50.269
                                                      62.157
                                                               76.500
                                                                         1.00
                                                                               40.14
               6719
      ATOM
                                            50.331
50.912
                      CE2
                          TYR B 120
                                                      64.116
                                                               77.855
                                                                         1.00
                                                                              38.09
      ATOM
               6720
                      CZ
                          TYR B 120
                                                                        1.00
                                                      63.301
                                                               76.933
                                                                              39.35
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46.154
                      OH
                          TYR B 120
                                                      63.654
                                                               76.448
                                                                         1.00
                                                                               44.06
      ATOM
               6722
                          VAL B 121
                      N
                                                               75.412
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                                                                        1.00
                                                                              31.03
      ATOM
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47.685
                      CA
                          VAL B 121
                                                      63.116
                                                               74.035
                                                                        1.00
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              6724
                     C
                          VAL B 121
                                                      64.176
                                                               73.750
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                                                               73.914
                          VAL B 121
                                            47.482
                                                      65.377
                                                                        1.00
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  20
              6726
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                          VAL B 121
                                            45.513
                                                      63.229
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                                            46.050
44.343
                     CG1
                          VAL B 121
                                                     62.953
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                                                                        1.00 33.17
      ATOM
              6728
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                          VAL B 121
                                                     62.275
63.701
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73.312
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              6729
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                          LYS B 122
                                            48.829
                                                                        1.00 29.19
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              6730
                     CA
                          LYS B 122
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                                                     64.558
                                                               73.126
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49.398
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                                                     65.317
                                                               71.807
                                                                        1.00 28.45
      ATOM
              6732
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                          LYS B 122
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                                                               70.791
                                                                        1.00 26.56
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              6733
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                              B 122
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                                                                        1.00 34.96
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                     CE
                          LYS B 122
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                                                              69.458
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     ATOM
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                         GLN B 123
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                                                              68.613
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              6746
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              6747
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                    CA
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                          TRP B 124
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                                                              71.783
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                          TRP
                                                     67.197
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                         TRP
                              B 124
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                         TRP
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                                           52.357
                                                                       1.00 23.47
             6757
6758
     ATOM
                    CE3
                         TRP
                              B 124
                                           53.667
                                                    68.703
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                                                                             21.99
     ATOM
                    CZ2
                         TRP
                              B 124
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                                                    70.420
                                                              65.934
                                                                       1.00
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                    CZ3
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52.144
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69.250
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72.030
                              B 124
                                                                       1.00
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             6760
                    CH2
                         TRP
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                                                                       1.00
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                         ARG B 125
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             6762
     ATOM
                    CA
                         ARG
                             B 125
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                         ARG
                             В
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72.220
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65
    ATOM
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                        ARG B
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55.721
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69.706
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             6772
                    N
                         HIS B
                               126
                                                             74.665
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             6773
                    CA
                        HIS B 126
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                        HIS B 126
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                                                                            24.67
    MOTA
             6775
                    0
                        HIS B 126
                                          52.905
                                                    69.909
                                                             76.857
                                                                       1.00
                                                                            25.37
70
             6776
    ATOM
                   СВ
                        HIS B 126
                                          55.651
                                                    71.374
                                                             76.453
                                                                       1.00 24.85
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	ATOM ATOM	6777 6778	CG NTD1	HIS B		57.160 57.956	71.401 72.073	76.540 75.629	1.00 25.08 1.00 27.14
	ATOM	6779		HIS B		58.009	70.775	77.387	1.00 23.78
	ATOM	6780		HIS B		59.227	71.897	75.944	1.00 24.80
5	MOTA	6781		HIS B		59.288	71.117	77.012	1.00 25.23
	ATOM	6782	N	SER B		53.066	70.394	74.693	1.00 24.40
	MOTA	6783 6784	CA	SER B		51.658 50.885	70.631 69.340	74.553 74.516	1.00 24.97 1.00 25.44
	ATOM ATOM	6785	С 0	SER B		51.376	68.316	74.076	1.00 25.17
10	ATOM	6786	CB	SER B		51.363	71.440	73.292	1.00 24.87
- 0	ATOM	6787	ŌĠ	SER B		52.058	70.913	72.165	1.00 22.76
	ATOM	6788	N	TYR B		49.674	69.409	75.033	1.00 27.02
	ATOM	6789	CA	TYR B		48.758	68.291	74.979	1.00 28.11
15	MOTA	6790	C	TYR B		47.368	68.716	75.343 75.838	1.00 28.88 1.00 28.25
15	ATOM ATOM	6791 6792	O CB	TYR B		47.150 49.187	69.827 67.168	75.907	1.00 28.23
	ATOM	6793	CG	TYR B		49.269	67.458	77.380	1.00 30.06
	ATOM	6794	CD1	TYR B	128	48.140	67.288	78.201	1.00 31.72
	ATOM	6795	CD2	TYR B	128	50.484	67.806	77.991	1.00 29.65
20	MOTA	6796	CE1		128	48.212	67.504	79.598	1.00 31.79
	ATOM	6797		TYR B		50.567	68.014	79.381	1.00 29.51
	ATOM ATOM	6798 6799	CZ OH		128 128	49.422 49.443	67.842 68.027	80.174 81.543	1.00 32.28 1.00 34.81
	ATOM	6800	N	THR B		46.442	67.791	75.112	1.00 29.01
25	ATOM	6801	CA	THR B		45.074	67.959	75.497	1.00 29.49
	MOTA	6802	С	THR B		44.674	66.844	76.495	1.00 29.76
	ATOM	6803	0	THR B		45.150	65.703	76.423	1.00 29.04
	ATOM	6804	CB	THR B		44.217 42.934	67.955 68.470	74.205 74.494	1.00 29.44 1.00 35.43
30	ATOM ATOM	6805 6806	OG1 CG2	THR B		43.907	66.606	73.732	1.00 33.43
50	ATOM	6807	N		130	43.812	67.195	77.440	1.00 30.39
	MOTA	6808	CA		130	43.297	66.238	78.387	1.00 30.28
	ATOM	6809	С	ALA B		41.922	66.613	78.895	1.00 31.10
2.5	MOTA	6810	0	ALA B		41.466	67.759	78.766	1.00 30.80
35	ATOM ATOM	6811 6812	CB N	ALA B SER B		44.253 41.282	66.136 65.620	79.585 79.517	1.00 30.74 1.00 31.93
	ATOM	6813	CA	SER B		40.089	65.826	80.321	1.00 31.96
	ATOM	6814	C	SER B		40.512	65.949	81.790	1.00 31.93
	ATOM	6815	0	SER B		41.546	65.445	82.162	1.00 32.28
40	ATOM	6816	CB		131	39.171	64.654	80.145	1.00 31.92
	ATOM ATOM	6817 6818	OG N	SER B	131	38.721 39.713	64.642 66.602	78.807 82.632	1.00 34.06 1.00 31.99
	ATOM	6819	CA	TYR B		40.099	66.805	84.018	1.00 32.05
	ATOM	6820	C	TYR B		38.923	66.642	84.977	1.00 32.91
45	ATOM	6821	0	TYR B		37.862	67.210	84.772	1.00 31.84
	ATOM	6822	CB	TYR B		40.716	68.214	84.203	1.00 31.57
	MOTA	6823	CG	TYR B		42.069 43.234	68.361 67.880	83.561	1.00 32.18 1.00 32.14
	ATOM ATOM	6824 6825		TYR B		42.192	68.925	82.304	1.00 32.14
50	ATOM	6826	CE1			44.496	67.990	83.547	1.00 33.68
	MOTA	6827	CE2	TYR B	132	43.426	69.018	81.666	1.00 33.56
	ATOM	6828	CZ	TYR B		44.561	68.561	82.290	1.00 32.85
	MOTA	6829	ОН	TYR B		45.734	68.690	81.622	1.00 34.63 1.00 35.04
55	ATOM ATOM	6830 6831	N CA	ASP B		39.121 38.138	65.872 65.818	86.033 87.102	1.00 37.05
33	ATOM	6832	C	ASP B		38.750	66.493	88.306	1.00 38.09
	ATOM	6833	ŏ	ASP B		39.942	66.770	88.326	1.00 38.74
	ATOM	6834	CB	ASP B	133	37.676	64.392	87.368	1.00 36.73
	MOTA	6835	CG	ASP B	133	36.605	63.965	86.384	1.00 38.46
60	ATOM	6836	OD1	ASP B	133	35.733	64.824	86.085	1.00 38.84
	ATOM ATOM	6837 6838	N N	ASP B		36.548 37.945	62.827 66.837	85.843 89.285	1.00 38.67 1.00 39.69
	ATOM	6839	CA	ILE B		38.499	67.440	90.495	1.00 41.09
	ATOM	6840	C	ILE B		37.970	66.675	91.691	1.00 43.16
65	ATOM	6841	0	ILE B	134	36.779	66.539	91.822	1.00 42.96
	ATOM	6842	CB	ILE B		38.134	68.914	90.615	1.00 40.24
	ATOM	6843		ILE B	134 134	38.732 38.650	69.685 69.461	89.449 91.936	1.00 39.46 1.00 39.97
	ATOM ATOM	6844 6845	CG2	ILE B		38.549	71.149	89.505	1.00 39.97
70	ATOM	6846	N	TYR B		38.867	66.176	92.542	1.00 45.80

	MOTA	6847	CA	TYR	B 135	38.4	35 65.37	4 93.714	1.00	48.11
	ATOM	6848	C	TYR	B 135	38.60	04 66.19			49.00
	ATOM	6849	0	TYR	В 135					48.31
	ATOM	6850	CB		В 135					
5	ATOM	6851			В 135					
	ATOM	6852			B 135					
	ATOM	6853			B 135		_			
	ATOM	6854			B 135					
	ATOM	6855		TIL	D 135					
10					B 135					53.21
10		6856			B 135				1.00	54.72
	ATOM	6857			B 135				1.00	54.58
	ATOM	6858			B 136		4 66.416	95.648		51.11
	ATOM	6859	CA	ASP	B 136	37.41				
	ATOM	6860	С	ASP	B 136					53.83
15	ATOM	6861	0	ASP	B 136	37.36	4 65.080			
	ATOM	6862	CB		B 136					52.71
	ATOM	6863	ĊĠ		B 136					
	ATOM	6864		ACD	B 136		3 60.308			51.80
	ATOM	6865	ODI	YGD	B 136		2 68.293			49.25
20	ATOM	6866		ASP	D 130				1.00	
20	ATOM		N		B 137				1.00	
		6867	CA		B 137				1.00	57.54
	ATOM	6868	C		в 137			100.917	1.00	59.20
	ATOM	6869	0		в 137		4 64.447	101.491	1.00	
	ATOM	6870	CB		B 137	41.11	2 65.852	99.718	1.00	
25	ATOM	6871	CG		B 137	41.97	2 65.236			58.13
	ATOM	6872	CD1	LEU	B 137	43.19			1.00	
	ATOM	6873	CD2	LEU	B 137	42.36				58.48
	ATOM	6874	N		B 138	38.42		101.415		
	ATOM	6875	CA	ACN	B 138	37.72				60.98
30	ATOM	6876	C		B 138			102.705		62.32
•	ATOM	6877	Õ		B 138	36.38		102.627		63.17
	ATOM	6878	CB			35.55		103.543		63.85
	ATOM			ASN	B 138	37.53		103.185		62.59
		6879	CG		B 138	38.69		104.046		63.40
25	ATOM	6880			В 138	38.57	5 68.746	105.268	1.00	64.31
35	ATOM	6881			B 138	39.82		103.411	1.00	63.58
	ATOM	6882			B 139	36.18	1 65.325	101.499		64.15
	ATOM	6883	CA	LYS	B 139	35.02	3 64.493	101.266		64.69
	ATOM	6884	С	LYS	B 139	35.53	2 63.413	100.320		65.21
	ATOM	6885	0	LYS	B 139	36.47	9 63.642	99.585		65.06
40	ATOM	6886	CB	LYS	в 139	33.92		100.590		64.96
	ATOM	6887	CG		B 139	33.72		101.069		
	ATOM	6888	CD		B 139	32.47				64.79
	ATOM	6889	CE		B 139	32.15		100.391	1.00	
	ATOM	6890	NZ		B 139		00.708	100.757		65.49
45	ATOM	6891				31.094		99.832		63.71
13	ATOM	6892	N		B 140	34.95	62.222	100.335		65.77
			CA		B 140	35.388		99.367	1.00	66.20
	ATOM	6893	C		B 140	34.682		98.038		64.94
	ATOM	6894	0		B 140		60.551	97.493	1.00	65.35
5 0	ATOM	6895	CB		B 140	34.966		99.807		67.02
50	MOTA	6896	CG	ARG	B 140	35.718	59.136	100.971		70.61
	ATOM	6897	CD	ARG	B 140	35.212		101.215		74.78
	ATOM	6898	NE	ARG	B 140	35.526	57.150	102.535	1 00	78.56
	ATOM	6899	CZ	ARG	B 140	36.668		102.863	1.00	
	ATOM	6900	NH1		B 140	37.656		101.977		
55	ATOM	6901			B 140	36.828		104.094	1.00	02.23
	ATOM	6902			B 141	34.756			1.00	
	ATOM	6903			B 141			97.508	1.00	
						33.921		96.353	1.00	
	ATOM	6904			B 141	34.563		95.163	1.00	59.88
60	ATOM	6905			В 141	35.290		95.317	1.00	58.49
60	ATOM	6906			в 141	32.731	63.889	96.821	1.00	62.00
	ATOM	6907			B 141	31.581		97.546	1.00	
	ATOM	6908	CD	GLN 1	B 141	30.365		97.737	1.00	
	ATOM	6909			3 141	30.518		97.718	1.00	
	ATOM	6910			3 141	29.172		97.909	1 00	CA 71
65	ATOM	6911			3 142	34.226			1.00	
	ATOM	6912			3 142	34.549		93.970	1.00	
	ATOM	6913			3 142			92.724	1.00	
	ATOM	6914				33.516		92.566	1.00	
					3 142	32.351		92.903	1.00	
70	ATOM	6915			3 142	34.439	62.983	91.546	1.00	57.42
70	ATOM	6916	CG :	LEU E	3 142	35.432	61.806	91.423	1.00	58.38

	ATOM	6917	CD1	LEU 1	B 142	34.881	60.708	90.505	1.00	58.70
	ATOM	6918	CD2	LEU I	R 142	36.823	62.241	90.928	1.00	57.90
										-
	ATOM	6919	N		B 143	33.910	66.251	92.096		54.79
	ATOM	6920	CA	ILE 1	3 143	32.892	67.270	91.892	1.00	54.52
5	ATOM	6921	С		3 143	32.236	66.971	90.554	1 00	53.58
,										
	ATOM	6922	0		3 143	32.897	66.682	89.568		53.27
	ATOM	6923	CB	ILE I	3 143	33.420	68.714	91.929	1.00	54.74
	ATOM	6924	CG1		3 143	33.846	69.140	90.543	1 00	55.65
										54.99
	ATOM	6925	CG2			34.528	68.876	92.987		
10	ATOM	6926	CD1	ILE 1	3 143	33.652	70.604	90.273	1.00	56.96
	ATOM	6927	N	THR 1	3 144	30.922	67.044	90.547	1.00	52.14
	ATOM	6928	CA	THR		30.130	66.662	89.410		51.43
	ATOM	6929	С	THR I		29.588	67.855	88.608		49.50
	ATOM	6930	0	THR I	3 144	29.032	67.663	87.546	1.00	49.43
15	ATOM	6931	CB	תאא ו	3 144	28.989	65.746	89.966	1 00	51.93
10						29.462	64.382	90.017		52.78
	MOTA	6932	OG1							
	ATOM	6933	CG2	THR I	3 144	27.758	65.689	89.053	1.00	53.08
	ATOM	6934	N	GLU I	3 145	29.791	69.075	89.099	1.00	47.72
	ATOM	6935		GLU I		29.212	70.284	88.490		46.86
	-		CA							
20	ATOM	6936	С	GLU I		30.290	71.195	87.943		44.59
	ATOM	6937	0	GLU I	3 145	31.366	71.145	88.421	1.00	42.44
	ATOM	6938	СВ	GLU I		28.497	71.160	89.547	1 00	46.71
	ATOM	6939	CG	GLU I		27.623	70.473	90.570		48.46
	ATOM	6940	$^{\mathtt{CD}}$	GLU I	3 145	26.846	71.497	91.401	1.00	50.31
25	ATOM	6941	OE1	GLU F	3 145	26.968	71.449	92.665	1.00	52.18
		6942	OE2	GLU I		26.156	72.368	90.784		46.09
	ATOM		_							
	ATOM	6943	N	GLU I	3 146	29.958	72.075	86.998		43.57
	ATOM	6944	CA	GLU H	3 146	30.931	73.056	86.481	1.00	42.81
	ATOM	6945	C	GLU E		32.323	72.410	86.287	1 00	40.46
20										39.08
30	ATOM	6946	0	GLU I		33.315	72.856	86.,852		
	ATOM	6947	CB	GLU F	3 146	31.052	74.245	87:454	1.00	43.05
	ATOM	6948	CG	GLU F	3 146	29.723	74.917	87.818	1.00	45.72
	ATOM	6949	CD	GLU I		28.904	75.360			46.80
	MOTA	6950		GLU E		29.471	75.547	85.539		47.90
35	MOTA	6951	OE2	GLU E	3 146	27.679	75.521	86.775	1.00	48.73
	ATOM	6952	N	ARG F	147	32.359	71.331	85.531	1.00	38.23
	ATOM	6953	CA	ARG E		33.580	70.611	85.318		37.89
	ATOM	6954	С	ARG E		34.416	71.336	84.280		35.94
	ATOM	6955	0	ARG I	3 147	33.909	71.963	83.342	1.00	36.10
40	ATOM	6956	CB	ARG E		33.302	69.182	84.821	1 00	38.26
10								85.866		40.91
	ATOM	6957	CG	ARG E		32.877	68.097			
	ATOM	6958	CD	ARG E	3 147	32.619	66.719	85.170		46.23
	ATOM	6959	NE	ARG F	3 147	31.968	65.683	85.989	1.00	50.43
	ATOM	6960	CZ	ARG E		32.447	64.445	86.217	1 00	53.41
4 =										
45	MOTA .	6961	NH1	ARG E		33.618	64.053	85.735		53.39
	ATOM	6962	NH2	ARG E	3 147	31.756	63.590	86.967	1.00	55.20
	ATOM	6963	N	ILE E	148	35.717	71.220	84.456	1.00	33.99
	ATOM	6964		ILE F		36.693		83.471		31.85
	MOTA	6965	С	ILE E		36.340	70.859	82.218		30.03
50	MOTA	6966	0	ILE E	148	36.159	69.669	82.298	1.00	28.67
	ATOM	6967	CB	ILE E	148	38.094	71.286	84.013	1.00	31.92
	ATOM	6968	CG1	ILE E		38.473	72.268	85.147		34.33
	ATOM	6969	CG2	ILE E		39.125	71.286	82.935		30.99
	ATOM	6970	CD1	ILE E	148	39.951	72.101	85.737	1.00	34.47
55	ATOM	6971	N	PRO E		36.240	71.484	81.062		28.84
55										
	ATOM	6972	CA	PRO E		35.799	70.742	79.884		28.65
	ATOM	6973	С	PRO E	149	36.804	69.738	79.409	1.00	28.89
	MOTA	6974	0	PRO E	149	37.980	69.796	79.776	1.00	28.38
		6975	ČВ	PRO E		35.601	71.820	78.802		28.36
	MOTA									
60	ATOM	6976	CG	PRO E		36.146	73.067	79.323	1.00	28.39
	ATOM	6977	CD	PRO E	149	36.544	72.892	80.760	1.00	29.09
	ATOM	6978	N	ASN E		36.318	68.799	78.614		29.51
	ATOM	6979	CA	ASN E		37.173	67.878	77.874		30.82
	ATOM	6980	C	ASN E	150	38.036	68.676	76.857	1.00	30.13
65	ATOM	6981	ō	ASN E		37.696	69.805	76.516		29.44
05										
	ATOM	6982	CB	ASN E		36.281	66.855	77.146		31.55
	MOTA	6983	CG	ASN E		35.515	65.954	78.114	1.00	37.05
	ATOM	6984		ASN E		35.879	65.831	79.298		36.83
	MOTA	6985		ASN E		34.467	65.304	77.616		45.68
70	MOTA	6986	N	ASN E	151	39.132	68.089	76.368	1.00	30.36

	ATOM ATOM ATOM	6988 6989	C	ASN ASN	ΙB		40.029 40.568 40.780	3 70.08	0 76.00	5 1.0	0 30.63 0 29.87 0 30.45
5	ATOM ATOM ATOM ATOM	6990 6991 6992 6993	CG OD:	ASN ASN L ASN 2 ASN	В В	151	39.323 38.593 39.228 37.273	3 69.14 7 67.94 8 66.98	0 74.09! 2 73.460 9 73.03:	5 1.0 5 1.0 3 1.0	0 31.24 0 33.32 0 38.87 0 33.94
10	ATOM ATOM ATOM ATOM	6994 6995 6996 6997	CA C	THR THR THR	В В	152 152 152 152	40.734 41.344 42.811 43.376	70.15 71.33 71.27	6 77.323 3 77.906 5 77.522	3 1.0 5 1.0 2 1.0	0 28.47 0 27.81 0 27.45
15	ATOM ATOM ATOM ATOM	6998 6999 7000 7001	CB OG1 CG2 N	THR THR	B B B	152 152 152 153	41.106 39.765 41.952 43.381	71.36 71.82 72.36	5 79.391 4 79.629 0 80.087	1.0 1.0 1.0	0 27.63
	ATOM ATOM ATOM ATOM	7002 7003 7004 7005	CA C O CB	GLN GLN	B B	153 153 153	44.743 45.821 46.979 44.750	72.586 72.836 72.52	5 76.699 5 77.764 7 77.573	1.00 1.00 1.00	0 27.91 0 28.03 0 27.08
20	ATOM ATOM ATOM ATOM	7006 7007 7008 7009	CG CD OE1 NE2	GLN GLN GLN	B B B	153 153	44.107 43.694 42.905	73.430 74.713 75.503	74.316 73.587 74.125	1.00 1.00 1.00	27.94 26.46 27.80 28.54
25	ATOM ATOM ATOM	7010 7011 7012	N CA C	TRP TRP TRP	B B B	154 154 154	44.242 45.430 46.316 45.476	73.462 73.658 73.969	78.862 79.961 81.180	1.00	
30	ATOM ATOM ATOM ATOM	7013 7014 7015 7016	O CB CG CD1		B B B	154 154 154	44.400 47.285 48.174 48.067	74.514 74.803 75.032 76.007	79.670 80.832	1.00	26.97 29.09 30.42 34.21
	ATOM ATOM ATOM ATOM	7017 7018 7019 7020	CD2 NE1 CE2 CE3	TRP TRP TRP	B B	154 154 154 154	49.260 49.043 49.794 49.849	74.221 75.865 74.765 73.080	82.711 82.399	1.00 1.00 1.00	29.80 34.81 33.62 31.67
35	ATOM ATOM ATOM ATOM	7021 7022 7023 7024	CZ2 CZ3 CH2 N	TRP TRP TRP VAL	B B	154 154 154 155	50.901 50.963 51.468 45.944	74.211 72.530 73.100 73.584	83.065 81.329 82.511	1.00 1.00 1.00	33.57 33.77 35.86
40	ATOM ATOM ATOM ATOM	7025 7026 7027 7028	CA C O CB	VAL VAL VAL	B B B	155 155 155	45.295 46.323 47.293	73.925 74.186 73.499	83.625 84.721 84.825	1.00 1.00 1.00	27.30 28.02 28.50 27.25
45	ATOM ATOM ATOM	7029 7030 7031	CG1 CG2 N	VAL VAL THR	B B B	155 155 155 156	44.468 43.605 43.669 46.050	72.766 73.290 72.012 75.109	84.254 85.381 83.259 85.605	1.00	28.49 27.80 29.00 29.64
	ATOM ATOM ATOM ATOM	7032 7033 7034 7035	CA C O CB	THR THR THR THR	B :	156 156	46.963 46.229 45.432 47.971	75.351 75.874 76.827 76.511	86.704 87.899 87.774 86.433	1.00	31.54 31.50 31.11 31.07
50	ATOM ATOM ATOM ATOM	7036 7037 7038 7039	CG2 N	THR THR TRP	В : В :	156 157	48.561 49.096 46.614 46.212	76.429 76.360 75.350 75.919	85.136 87.335 89.058 90.344	1.00 1.00 1.00	37.41 31.91 32.16
55	ATOM ATOM ATOM ATOM	7040 7041 7042 7043	С О СВ	TRP TRP TRP	B 1 B 1 B 1	L57 L57 L57	46.976 48.056 46.644	77.210 77.340 74.988	90.519 89.997 91.509	1.00 1.00 1.00	32.69 33.37 33.68 32.93
60	ATOM ATOM ATOM	7044 7045 7046	CD1 CD2 NE1	TRP TRP TRP	B 1 B 1 B 1	L57 L57 L57	45.962 46.539 44.597 45.618	73.635 72.441 73.371 71.434	91.559 91.353 91.906 91.530	1.00	30.74 28.69 28.30 31.58
	ATOM ATOM ATOM	7047 7048 7049 7050	CE3 CZ2	TRP 1 TRP 1 TRP 1 TRP 1	B 1 B 1	.57 .57	44.412 43.497 43.171 42.268	71.993 74.180 71.385 73.581	91.857 92.225 92.105 92.485	1.00 1.00 1.00	29.40 34.40 34.85
65	ATOM ATOM ATOM	7051 7052 7053	CH2 N CA	TRP I SER I SER I	3 1 3 1 3 1	.57 .58 .58	42.117 46.419 47.129	72.194 78.156 79.373	92.423 91.268 91.686	1.00 1.00 1.00	34.99 35.01 34.79 34.84
70	ATOM ATOM ATOM	7054 7055 7056	0	SER E SER E SER E	3 1	58	48.159 48.094 46.148	78.893 77.783 80.317	92.697 93.110 92.351	1.00	34.81 34.12 35.28

	ATOM	7057	OG			158		5.236	79.558	93.138		35.00
	ATOM	7058	N			159 159		9.135	79.690 79.190	93.062 93.919		35.67 36.90
	ATOM ATOM	7059 7060	CA C			159		9.799	78.909	95.352		
5	ATOM	7061	Ö		_	159		0.799	78.066	96.000		39.07
,	ATOM	7062	СВ			159		1.263	80.288	93.848		36.48
	ATOM	7063	CG			159		0.882	81.140	92.744		36.04
	ATOM	7064	CD			159		3.373	81.072	92.635		36.34
	ATOM	7065	N	VAL		160		3.787	79.601	95.844		39.52
10	ATOM	7066	CA	VAL		160		3.314	79.362	97.192		39.85
	ATOM	7067	С	VAL		160	46	5.849	79.215	96.995	1.00	39.62
	MOTA	7068	0	VAL	В	160	46	5.318	79.748	96.043	1.00	40.31
	MOTA	7069	CB	VAL	В	160	48	3.616	80.549	98.116		40.71
	ATOM	7070	CG1	VAL	В	160		140	80.769	98.235		41.63
15	ATOM	7071	CG2			160		7.946	81.801	97.605		41.78
	ATOM	7072	N	GLY		161		.194	78.435	97.832		38.75
	MOTA	7073	CA	GLY		161		1.758	78.307	97.765		38.17
	ATOM	7074	C	GLY		161		.285	77.225	96.830		37.54
20	MOTA	7075	0	GLY		161		.794	76.100	96.821		36.68
20	ATOM ATOM	7076 7077	N CA	HIS HIS		162 162		243	77.543 76.559	96.076 95.160		36.80 36.56
	ATOM	7078	CA	HIS		162		957	77.155	93.993		34.81
	ATOM	7079	Ö	HIS		162		067	76.508	93.466		34.79
	ATOM	7080	СВ	HIS		162		902	75.554	95.938		37.14
25	ATOM	7081	CG			162		770	76.177	96.682		40.25
	ATOM	7082		HIS		162		.455	75.837	97.977		42.53
	ATOM	7083		HIS		162		.872	77.118	96.309		42.08
	ATOM	7084	CE1	HIS	В	162	39	.415	76.548	98.376	1.00	43.68
	ATOM	7085	NE2	HIS	В	162	39	.042	77.332	97.382	1.00	44.43
30	ATOM	7086	N	LYS	В	163		.272	78.387	93.604		33.74
	ATOM	7087	CA	LYS		163		.727	78.953	92.370		34.09
	ATOM	7088	C	LYS		163		.340	78.168	91.224		32.87
	ATOM	7089	0_	LYS		163		.407	77.657	91.394		32.77
25	ATOM	7090	CB		В	163		.114	80.411	92.173		34.03
35	ATOM	7091	CG	LYS		163		.512	81.400	93.157		34.96
	ATOM	7092 7093	CD	LYS LYS		163		.055	82.788 83.843	92.797 93.846		34.44 34.13
	ATOM ATOM	7093	CE NZ	LYS		163 163		.162	85.145	93.358		30.81
	ATOM	7095	N	LEU				.635	78.028	90.107		32.21
40	ATOM	7096	CA	LEU				.143	77.331	88.918		32.26
10	ATOM	7097	C	LEU				.058	78.224	87.703		30.77
	ATOM	7098	Ō	LEU				.179	79.059	87.588		30.09
	ATOM	7099	CB	LEU	В	164	41	.308	76.107	88.570	1.00	32.35
	ATOM	7100	CG	LEU		164		.380	74.840	89.397		35.85
45	MOTA	7101		LEU		164		.073	74.031	89.319		37.85
	ATOM	7102		LEU		164		.499	73.968	88.980		37.12
	ATOM	7103	N	ALA				.982	78.018	86.789		29.97
	ATOM	7104	CA					.969	78.719	85.527		29.70
EΛ	ATOM	7105	C	ALA				.264 .157	77.683 76.845	84.452 84.621		29.05 29.22
50	ATOM ATOM	7106 7107	O CB	ALA ALA				. 985	79.805	85.522		29.61
	ATOM	7107	N	TYR				.503	77.720	83.371		27.94
	ATOM	7100	CA	TYR				.702	76.775	82.286		27.80
	ATOM	7110	C	TYR				.479	77.394	80.911		27.07
55	ATOM	7111	ŏ	TYR				.950	78.492	80.773		26.60
	ATOM	7112	СB	TYR				.811	75.548	82.478		28.31
	ATOM	7113	CG	TYR	В	166		.313	75.795	82.488		28.99
	MOTA	7114	CD1	TYR	В	166	39	. 598	75.876	81.296		31.31
	MOTA	7115	CD2	TYR	В	166		.607	75.893	83.680		30.82
60	MOTA	7116	CE1	TYR				. 228	76.073	81.273		31.44
	MOTA	7117	CE2					.204	76.077	83.669		33.40
	MOTA	7118	CZ	TYR				.528	76.179	82.450		31.55
	ATOM	7119	ОН	TYR				.150	76.348	82.390		30.35
. -	ATOM	7120	N	VAL				.945	76.692	79.901		26.39
65	MOTA	7121	CA	VAL				.799	77.133	78.540		26.34
	ATOM	7122	C	VAL				.038	76.045	77.759		25.99
	ATOM ATOM	7123 7124	O CB	VAL VAL				.388 .171	74.866 77.442	77.788 77.908		25.38 26.71
	ATOM	7124	CB CG1	VAL				.041	77.790	76.447		27.08
70	ATOM	7126		VAL				.858	78.584	78.671		26.78
-					_							•

5	ATOM	7128 7129 7130 7131 7132	CA T C T O T CB T CG T	RP B RP B RP B RP B	168 168 168 168 168	40.993 40.125 39.689 39.330 38.953 37.956	75.616 76.403 77.566 75.181	76.311 75.089 75.176 77.160	1.00 26.65 1.00 26.23 1.00 25.50
10	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	7133 7134 7135 7136 7137 7138 7139	CD2 T NE1 T CE2 T CE3 T CZ2 T	RP B	168 168 168 168	37.991 36.758 36.886 36.106 36.154 34.909	72.940 74.723 72.499 73.570 75.962 73.622	76.290 75.782 75.599 75.287 75.588 74.602	1.00 28.41 1.00 29.22 1.00 29.45 1.00 28.79 1.00 31.73 1.00 30.76
15	ATOM ATOM ATOM ATOM ATOM	7140 7141 7142 7143 7144	CH2 TI N AS CA AS C AS	RP B SN B SN B SN B	168 169 169 169	34.949 34.354 39.801 39.676 40.469 40.011	76.013 74.847 75.765 76.441 77.741 78.742	74.909 74.403 73.938 72.636 72.552 71.976	1.00 31.40 1.00 31.36 1.00 27.78 1.00 28.42 1.00 27.41 1.00 26.62
20	ATOM ATOM ATOM ATOM ATOM	7145 7146 7147 7148 7149	CB AS CG AS OD1 AS ND2 AS	N B N B N B	169 169 169 169	38.225 37.588 36.440 38.351	76.603 75.267 75.203 74.219	72.239 71.844 71.546 71.858	1.00 29.40 1.00 31.42 1.00 37.40 1.00 33.37
25	ATOM ATOM ATOM ATOM	7150 7151 7152 7153	CA AS C AS O AS CB AS	NB NB NB	170	41.674 42.621 42.273 42.907 42.833	77.710 78.822 80.047 81.088 79.246	73.127 73.013 73.808 73.635 71.542	1.00 25.57 1.00 25.04 1.00 24.12 1.00 23.07 1.00 25.51
30	ATOM ATOM ATOM ATOM ATOM	7154 7155 7156 7157 7158	OD1 AS ND2 AS N AS	NB:	171	43.671 43.598 44.494 41.255 40.908	78.250 77.047 78.766 79.942 81.025	70.742 70.953 69.848 74.653 75.535	1.00 25.77 1.00 26.32 1.00 23.45 1.00 24.36
35	ATOM ATOM ATOM	7159 7160 7161 7162	C AS O AS CB AS CG AS	P B 1 P B 1 P B 1 P B 1	171 171 171 171	41.116 41.075 39.461 39.282	80.625 79.450 81.451 82.398	76.984 77.342 75.322 74.138	1.00 25.01 1.00 25.77 1.00 25.33 1.00 25.44 1.00 26.23
40	ATOM ATOM ATOM ATOM ATOM ATOM	7163 7164 7165 7166 7167 7168	CA IL	P B 1	L71 L72 L72 L72	40.006 38.398 41.265 41.503 40.224 39.430	83.402 82.225 81.642 81.463 81.567 82.447	73.973 73.322 77.828 79.254 80.042 79.780	1.00 26.67 1.00 31.72 1.00 26.70 1.00 26.99 1.00 27.13
45	ATOM ATOM ATOM ATOM ATOM	7169 7170 7171 7172	CB IL CG1 IL CG2 IL CD1 IL	E B 1 E B 1 E B 1 E B 1 R B 1	.72 .72 .72 .72	42.443 43.694 42.748 44.628 40.053	82.577 82.571 82.479 83.682 80.672	79.780 79.733 78.891 81.268 79.203 81.002	1.00 28.16 1.00 27.38 1.00 26.31 1.00 27.37 1.00 28.62
50	ATOM ATOM ATOM ATOM ATOM	7174 7175 7176 7177	CA TY C TY C TY CB TY	R B 1 R B 1 R B 1 R B 1	.73 .73 .73 .73	38.939 39.487 40.559 38.030 37.340	80.689 80.600 80.022 79.479	81.944 83.336 83.545 81.753	1.00 27.60 1.00 29.16 1.00 29.79 1.00 27.70 1.00 29.36
55	ATOM ATOM ATOM ATOM ATOM	7179 7180 7181 7182	CD1 TY CD2 TY CE1 TY CE2 TY	8 B 1 8 B 1 8 B 1 8 B 1	.73 .73 .73 .73	38.031 36.007 37.417 35.357	79.485 79.156 79.862 79.173 79.866	80.431 79.289 80.321 78.037 79.070	1.00 29.61 1.00 29.96 1.00 30.68 1.00 31.87 1.00 30.15
60	ATOM ATOM ATOM ATOM	7184 6 7185 7 7186 6 7187 6	OH TYI N VAI CA VAI C VAI	B 1 B 1 B 1 B 1	73 74 74 74	36.081 35.514 38.728 39.111 37.983	79.514 79.553 81.139 81.074 80.538	77.935 76.692 84.295 85.697 86.587	1.00 29.94 1.00 28.17 1.00 31.23 1.00 33.00 1.00 34.12
65	ATOM ATOM ATOM ATOM ATOM ATOM	7189 (7190 (7191 (7192)		B 1	74 74 75	36.816 39.546 39.769 40.807 38.343	80.912 82.482 82.455 82.954 79.641	86.412 86.223 87.736 85.556 87.508	1.00 34.28 1.00 33.90 1.00 34.58 1.00 32.03 1.00 34.69
70	ATOM ATOM ATOM	7194 (7195 (C LYS	B 1' B 1' B 1'	75 75	37.430 37.968 39.108 37.365	79.108 79.489 79.152 77.602	88.522 89.872 90.204 88.501	1.00 35.51 1.00 36.26 1.00 36.45 1.00 35.81

	ATOM ATOM ATOM	7197 7198 7199	CG CD CE	LYS E LYS E	175	36.352 36.367 34.990	77.025 75.511 74.962	87.516 87.545 87.372	1.00 1.00 1.00	40.55
5	ATOM ATOM ATOM	7200 7201 7202	NZ N CA	LYS E	3 175 3 176	34.425 37.159 37.528	74.585 80.204 80.636	88.683 90.641 91.986	1.00 1.00	
	ATOM ATOM ATOM	7203 7204 7205	C O CB	ILE E	176 176	37.298 38.066 36.680	79.471 79.265 81.832	92.909 93.823 92.399	1.00	37.45 37.82 38.10
10	ATOM ATOM ATOM ATOM	7206 7207 7208 7209	CG1 CG2 CD1 N	ILE E	176 176	37.003 36.865 38.466 36.251	83.028 82.178 83.421 78.680	91.494 93.913 91.501 92.681	1.00	38.17 38.95 38.95 37.61
15	ATOM ATOM ATOM	7210 7211 7211 7212	CA C	GLU E	177 177	36.050 35.825 35.155	77.476 76.353 76.515	93.498 92.567 91.548	1.00 1.00	37.49 36.65 36.82
	ATOM ATOM ATOM	7213 7214 7215	CB CG CD	GLU E	177 177	34.821 34.924 36.037	77.561 78.567 78.220	94.427 95.558 96.501	1.00 1.00 1.00	38.49 39.23 41.78
20	ATOM ATOM ATOM ATOM	7216 7217 7218 7219	OE1 OE2 N CA		177 178	36.325 36.617 36.378 36.235	77.003 79.160 75.208 74.018	96.632 97.099 92.899 92.057	1.00 1.00	41.29 42.97 36.33 36.94
25	ATOM ATOM ATOM	7220 7221 7222	C O CB	PRO B PRO B PRO B	178 178 178	34.832 34.718 36.723	73.724 73.336 72.900	91.518 90.354 92.968	1.00 1.00 1.00	37.41 37.02 36.73
30	ATOM ATOM ATOM ATOM	7223 7224 7225 7226	CG CD N CA	PRO B PRO B ASN B ASN B	178 179	37.755 37.212 33.781 32.448	73.585 74.954 73.905 73.518	93.833 94.079 92.303 91.833	$1.00 \\ 1.00$	36.47 36.06 38.31 39.69
50	ATOM ATOM ATOM	7227 7228 7229	C O CB	ASN B ASN B ASN B	179 179	31.625 30.432 31.676	74.684 74.529 72.810	91.033 91.289 91.004 92.942	1.00 1.00	40.15 39.85 40.15
35	ATOM ATOM	7230 7231 7232	ND2	ASN B ASN B	179 179	31.533 32.178 30.710	73.674 74.721 73.250	94.150 94.250 95.085	1.00 1.00	47.94
40	ATOM ATOM ATOM ATOM	7233 7234 7235 7236	N CA C O	LEU B LEU B LEU B	180 180 180	32.249 31.520 31.829 32.855	75.844 76.966 77.257 76.849	91.112 90.547 89.073 88.543	1.00 1.00	40.56 39.05 38.39
	ATOM ATOM ATOM	7237 7238 7239 7240		LEU B LEU B LEU B	180 180	31.756 30.847 29.368 31.318	78.219 78.321 77.967 77.406	91.388 92.619 92.302 93.714	$1.00 \\ 1.00$	41.21 45.88 48.11 49.70
45	ATOM ATOM ATOM	7241 7242 7243	N CA C	PRO B PRO B PRO B	181 181	30.898 31.084 32.383	77.926 78.337 79.071	88.410 87.028 86.845	1.00 1.00	37.96 37.59 37.17
50	ATOM ATOM ATOM	7244 7245 7246	O CB CG	PRO B PRO B	181 181	32.809 29.931 28.822	79.808 79.331 78.824	87.757 86.799 87.747	1.00 1.00	37.40 37.51 38.58
	ATOM ATOM ATOM ATOM	7247 7248 7249 7250	CD N CA C	PRO B SER B SER B	182 182	29.563 32.991 34.188 33.842	78.287 78.923 79.663 81.037	88.921 85.680 85.416 84.885	$1.00 \\ 1.00$	38.00 35.56 35.61 35.09
55	ATOM ATOM ATOM	7251 7252 7253	O CB OG	SER B SER B SER B	182 182	32.775 35.081 34.295	81.257 78.928 78.443	84.368 84.406 83.364	1.00	34.78 35.34 37.20
60	ATOM ATOM	7254 7255 7256	N CA C	TYR B TYR B TYR B	183 183	34.780 34.688 35.520	81.958 83.262 83.177	85.037 84.450 83.193	$1.00 \\ 1.00$	34.82 34.50 33.68
	ATOM ATOM ATOM ATOM	7257 7258 7259 7260	O CB CG CD1	TYR B TYR B TYR B	183 183	36.659 35.278 34.510 34.860	82.720 84.328 84.382 83.564	83.241 85.396 86.676 87.718	1.00 1.00	33.67 35.09 34.39 34.06
65	MOTA MOTA MOTA	7261 7262 7263	CD2 CE1 CE2	TYR B TYR B TYR B	183 183 183	33.369 34.154 32.648	85.201 83.556 85.219	86.807 88.869 87.973	1.00 1.00 1.00	34.61 36.35 35.36
70	ATOM ATOM ATOM	7264 7265 7266	CZ OH N	TYR B TYR B ARG B	183	33.040 32.365 34.949	84.377 84.337 83.589	89.003 90.187 82.063	1.00 1.00 1.00	40.21

	ATOM ATOM ATOM ATOM	7267 7268 7269 7270	B C ARG B 184 B O ARG B 184	35.686 36.505 35.964 34.723	84.877 85.932	80.728 80.829	1.00 31.81 1.00 33.62
5	ATOM ATOM ATOM ATOM	7271 7272 7273 7274	CG ARG B 184 CD ARG B 184 NE ARG B 184	35.402 34.642 35.371 34.838	83.574 82.835 82.777	78.268 77.197 75.937	1.00 33.23 1.00 32.80 1.00 34.26
10	ATOM ATOM ATOM ATOM	7275 7276 7277 7278	NH1 ARG B 184 NH2 ARG B 184 N ILE B 185	33.574 35.573 37.805 38.656	82.000 82.370 84.791	74.699 73.698 80.511	1.00 32.08 1.00 27.82 1.00 31.72
15	ATOM	7279 7280 7281 7282	O ILE B 185 CB ILE B 185 CG1 ILE B 185	38.925 38.971 40.019 39.806	86.496 87.704 85.616	79.087	1.00 30.73 1.00 31.11
20	ATOM ATOM ATOM ATOM ATOM	7283 7284 7285 7286 7287	CD1 ILE B 185 N THR B 186 CA THR B 186	40.951 39.150 39.202 39.437	86.815 85.829 85.604 86.022	81.252 83.580 78.127 76.753	1.00 28.61 1.00 30.91 1.00 29.74 1.00 28.74
25	ATOM ATOM ATOM ATOM	7288 7289 7290 7291	O THR B 186 CB THR B 186 OG1 THR B 186	38.360 37.757 40.792 40.892	85.490 84.466 85.552 84.098	75.845 76.158 76.208 76.217	1.00 29.54 1.00 28.68 1.00 29.21 1.00 24.81
23	ATOM ATOM ATOM ATOM	7292 7293 7294 7295	CG2 THR B 186 N TRP B 187 CA TRP B 187 C TRP B 187	41.922 38.169 37.138 37.680	86.169 85.801 85.721	77.084 74.710 73.715 72.313	1.00 28.72 1.00 30.37 1.00 31.00 1.00 30.96
30		7296 7297 7298 7299	O TRP B 187 CB TRP B 187 CG TRP B 187 CD1 TRP B 187	36.917 36.000 35.306 35.733	85.495 86.840 86.910 87.586	71.378 73.734 75.049 76.161	1.00 31.78 1.00 31.13 1.00 33.04 1.00 34.11
35	ATOM ATOM ATOM ATOM	7300 7301 7302	CD2 TRP B 187 NE1 TRP B 187 CE2 TRP B 187 CE3 TRP B 187	34.077 34.841 33.816 33.173	86.271 87.400 86.600 85.440	75.420 77.191 76.757 74.756	1.00 37.07 1.00 36.25 1.00 37.19 1.00 41.52
40	ATOM ATOM ATOM ATOM	7303 7304 7305 7306 7307	CZ2 TRP B 187 CZ3 TRP B 187 CH2 TRP B 187 N THR B 188 CA THR B 188	32.696 32.047 31.823 38.992 39.627	86.135 84.987 85.338 85.913 85.973	77.441 75.435 76.768 72.155	1.00 41.86 1.00 41.77 1.00 42.71 1.00 30.36
45	ATOM ATOM ATOM ATOM	7308 7309 7310 7311	C THR B 188 O THR B 188 CB THR B 188 OG1 THR B 188	40.291 40.908 40.730 41.580	84.686 84.651 87.063 86.859	70.866 70.424 69.373 70.897 72.032	1.00 30.00 1.00 30.49 1.00 30.70 1.00 30.29 1.00 27.37
	ATOM ATOM ATOM ATOM	7312 7313 7314 7315	CG2 THR B 188 N GLY B 189 CA GLY B 189 C GLY B 189	40.137 40.236 40.882 40.409	88.460 83.654 82.406 81.863	71.127 71.241 70.897 69.560	1.00 30.50 1.00 30.99 1.00 31.24
50	ATOM ATOM ATOM ATOM	7316 7317 7318 7319	O GLY B 189 N LYS B 190 CA LYS B 190 C LYS B 190	39.223 41.354 41.038 42.166	81.866 81.388 80.824 79.864	69.272 68.757 67.452 67.015	1.00 32.02 1.00 30.37 1.00 33.66 1.00 35.04
55	ATOM ATOM ATOM ATOM	7320 7321 7322 7323	O LYS B 190 CB LYS B 190 CG LYS B 190 CD LYS B 190	43.356 40.775 40.545 39.917	80.221 81.942 81.428 82.506	66.913 66.429 65.018	1.00 34.99 1.00 34.01 1.00 35.38 1.00 39.53
60	ATOM ATOM ATOM ATOM	7324 7325 7326 7327	CE LYS B 190 NZ LYS B 190 N GLU B 191 CA GLU B 191	38.972 37.900 41.757 42.682	81.861 82.816 78.640	64.075 63.027 62.564 66.750	1.00 44.37 1.00 45.44 1.00 48.69 1.00 34.96
65	ATOM ATOM ATOM ATOM	7328 7329 7330 7331	C GLU B 191 O GLU B 191 CB GLU B 191 CG GLU B 191	43.711 43.358 41.892 42.602	77.580 78.047 78.723 76.365 75.042	66.441 65.399 64.444 65.968 66.131	1.00 35.61 1.00 34.46 1.00 33.49 1.00 36.18 1.00 41.19
	ATOM ATOM ATOM ATOM	7332 7333 7334 7335	CD GLU B 191 OE1 GLU B 191 OE2 GLU B 191 N ASP B 192	41.692 40.903 41.745 44.975	73.861 73.401 73.415 77.691	65.794 66.674 64.639 65.646	1.00 41.19 1.00 45.56 1.00 48.35 1.00 44.81 1.00 32.21
70	ATOM	7336	CA ASP B 192	46.138	78.031	64.851	1.00 32.21

	MOTA MOTA	7337 7338	C O	ASP	В	192	46.318 47.166	79.485 79.810	64.541 63.752	1.00	
	ATOM ATOM	7339 7340	CB CG	ASP ASP			46.128 46.167	77.279 75.799	63.514 63.694	1.00	
5	ATOM	7341		ASP			46.877	75.306	64.610		36.83
	ATOM	7342	OD2	ASP	В	192	45.483	75.055	62.999		34.81
	ATOM	7343	N	ILE			45.587	80.375	65.181		29.66
	ATOM ATOM	7344 7345	CA C	ILE			45.702 45.914	81.777 82.678	64.823 66.028	1.00	
10	ATOM	7345	o	ILE			46.898	83.399	66.073	1.00	
	ATOM	7347	ČВ	ILE			44.461	82.220	64.029		30.62
	ATOM	7348	CG1				44.373	81.433	62.728		32.28
	ATOM	7349	CG2				44.520	83.749	63.742	1.00	
15	ATOM ATOM	7350 7351	CD1 N	ILE			43.175 44.987	81.840 82.671	61.855 66.983	1.00	36.86 27.43
13	ATOM	7352	CA	ILE			45.150	83.474	68.181	1.00	
	ATOM	7353	C	ILE			45.266	82.551	69.399	1.00	26.62
	ATOM	7354	0	ILE			44.393	81.732	69.652	1.00	
20	ATOM	7355	CB	ILE			43.959	84.369	68.414		27.86
20	ATOM ATOM	7356 7357	CG1 CG2				43.729 44.093	85.381 85.053	67.267 69.769		27.98 29.81
	ATOM	7358	CD1				44.845	86.329	66.950		28.45
	ATOM	7359	N	TYR			46.318	82.722	70.182		25.71
	MOTA	7360	CA	TYR			46.555	81.858	71.340		25.32
25	ATOM	7361	C	TYR			46.614	82.683	72.678		24.78
	ATOM ATOM	7362 7363	O CB	TYR TYR			47.474 47.889	83.517 81.158	72.868 71.161	1.00	
	ATOM	7364	CG	TYR			48.147	80.261	69.958		25.25
	ATOM	7365	CD1				48.509	80.777	68.722	1.00	28.88
30	ATOM	7366	CD2	TYR			48.154	78.870	70.095		28.51
	MOTA	7367	CE1	TYR TYR			48.798 48.470	79.928 78.012	67.627 69.003		27.62 25.69
	ATOM ATOM	7368 7369	CE2 CZ	TYR			48.470	78.552	67.803	1.00	
	ATOM	7370	OH	TYR			49.089	77.704	66.769		32.98
35	ATOM	7371	N	ASN			45.692	82.444	73.598	1.00	24.41
	ATOM	7372	CA	ASN			45.674	83.183	74.834	1.00	
	ATOM ATOM	7373 7374	C	ASN ASN			46.053 45.365	82 200 81 220	75.937 76.188	1.00	
	ATOM	7375	O CB	ASN			44.295	83.796	75.145	1.00	
40	ATOM	7376	CG	ASN			43.853	84.855	74.119	1.00	23.79
	MOTA	7377		ASN			44.404	85.941	74.062	1.00	
	ATOM	7378	ND2			196	42.810	84.547	73.364		22.39
	MOTA MOTA	7379 7380	N CA	GLY GLY		197	47.150 47.525	82.476 81.669	76.599 77.745		25.39 26.17
45	ATOM	7381	C	GLY		197	48.212	80.378	77.422	1.00	
	MOTA	7382	Ö	GLY		_	48.519	79.637	78.356		26.86
	MOTA	7383	N	ILE			48.366	80.086	76.132		24.30
	ATOM	7384	CA	ILE :			49.213				23.97 24.02
50	ATOM ATOM	7385 7386	C O	ILE :			50.078 49.754	79.547 80.607	74.521 73.954		24.02
50	ATOM	7387	СВ	ILE			48.418	77.790	75.190		24.16
	ATOM	7388	CG1	ILE :	В	198	47.310	78.236	74.222	1.00	24.52
	MOTA	7389		ILE :			47.891	76.975	76.389		21.53
55	ATOM ATOM	7390 7391		ILE I			46.628 51.169	77.132 78.836	73.499 74.224		24.60 23.15
33	ATOM	7391	N CA	THR			52.122	79.176	73.192		23.42
	ATOM	7393	C	THR			51.810	78.461	71.870		23.55
	MOTA	7394	0	THR :			51.195	77.390	71.840		24.28
	ATOM	7395	CB	THR			53.529	78.742	73.589		23.42
60	MOTA	7396	OGI	THR I	8	199	53.536 54.047	77.336 79.528	73.944 74.858		22.03
	ATOM ATOM	7397 7398	N	ASP I			52.223	79.528	70.786		23.33
	ATOM	7399	CA	ASP			52.202	78.499	69.449		24.01
	MOTA	7400	С	ASP :	В	200	53.425	77.600	69.345	1.00	23.87
65	ATOM	7401	0	ASP			54.156	77.393	70.346		23.48
	ATOM ATOM	7402 7403	CB CG	ASP :			52.193 53.550	79.595 80.189	68.384 68.127		24.16 24.91
	ATOM	7403		ASP :			54.429	80.171	69.033		20.58
	MOTA	7405		ASP			53.835	80.661	67.004		29.25
70	MOTA	7406	N	TRP	В	201	53.697	77.095	68.150		23.54

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	ATOM ATOM ATOM	740 740	8 C TRP B 2 9 O TRP B 2	201 56.192 201 56.952	76.577	67.970 68.302 68.941	1.00 23.29
5	ATOM ATOM ATOM ATOM	741	1 CG TRP B 2 2 CD1 TRP B 2	201 55.590 201 55.150	74.325 73.069	66.543 66.446 66.497	1.00 22.81 1.00 21.22 1.00 21.30
10	ATOM ATOM	7414 7414 7416 7416	4 NE1 TRP B 2 5 CE2 TRP B 2 6 CE3 TRP B 2	56.196 01 57.360 01 58.031	72.182 72.884 75.183	66.374 66.423 66.346 66.257	1.00 20.03 1.00 19.91 1.00 22.09
15	ATOM ATOM ATOM ATOM	7418 7419 7420 7421	B CZ3 TRP B 2 B CH2 TRP B 2 D N VAL B 2 L CA VAL B 2	01 59.367 01 59.664	72.429 74.732 73.368 77.752 78.137	66.245 66.168 66.164 67.853 68.096	1.00 20.94 1.00 22.14 1.00 21.14 1.00 22.90 1.00 23.28
20	ATOM ATOM ATOM	7422 7423 7424 7425	O VAL B 2 CB VAL B 2 CG1 VAL B 2	02 58.149 02 59.209 02 58.464 02 59.617	78.500 78.256 79.422 79.138	69.531 70.034 67.415 66.585	1.00 22.71 1.00 21.85 1.00 23.30 1.00 25.16
20	ATOM ATOM ATOM ATOM	7426 7427 7428 7429	N TYR B 20 CA TYR B 20 C TYR B 20	03 57.207 03 57.253 03 57.235	80.287 79.244 79.597 78.382	66.869 70.097 71.521 72.441	1.00 24.41 1.00 22.28 1.00 22.69 1.00 23.05
25	ATOM ATOM ATOM ATOM	7430 7431 7432 7433	CB TYR B 20 CG TYR B 20 CD1 TYR B 20	03 56.134 03 56.503 03 56.306	78.381 80.561 82.031 82.719	73.477 71.893 71.761 70.585	1.00 23.40 1.00 21.84 1.00 23.10 1.00 23.62
30	ATOM ATOM ATOM ATOM ATOM	7434 7435 7436 7437 7438	CE1 TYR B 20 CE2 TYR B 20 CZ TYR B 20	56.674 57.466 57.239	82.726 84.078 84.042 84.720	72.834 70.473 72.728 71.559	1.00 24.96 1.00 25.42 1.00 25.18 1.00 27.71
35	ATOM ATOM ATOM ATOM	7439 7440 7441 7442	OH TYR B 20 N GLU B 20 CA GLU B 20 C GLU B 20 O GLU B 20	04 56.503 04 56.475 04 57.839	86.039 77.326 76.160 75.592 75.359	71.495 72.081 72.952 72.942	1.00 22.52 1.00 22.72 1.00 23.42
40	ATOM ATOM ATOM ATOM	7443 7444 7445 7446	CB GLU B 20 CG GLU B 20 CD GLU B 20 OE1 GLU B 20	04 55.493 04 55.757 04 54.720	75.067 73.681 72.602 72.876	73.972 72.477 73.076 72.726 72.147	1.00 24.10 1.00 22.71 1.00 21.04 1.00 19.46
	ATOM ATOM ATOM ATOM	7447 7448 7449 7450	OE2 GLU B 20 N GLU B 20 CA GLU B 20 C GLU B 20	54.950 55 58.338 5 59.547	71.438 75.393 74.638 75.418	73.026 71.734 71.544	1.00 20.21 1.00 18.42 1.00 23.62 1.00 23.72
45	ATOM ATOM ATOM ATOM	7451 7452 7453 7454	O GLU B 20 CB GLU B 20 CG GLU B 20 CD GLU B 20	5 61.733 5 59.516 5 60.709	74.886 74.049 73.231	71.788 72.425 70.129 69.668	1.00 24.81 1.00 23.39 1.00 23.14 1.00 23.21
50	ATOM ATOM ATOM ATOM	7455 7456 7457 7458	OE1 GLU B 20 OE2 GLU B 20 N GLU B 20 CA GLU B 20	5 60.159 5 62.186 6 60.946	71.992 71.490 71.535 76.639 77.361	70.499 71.251 70.418 71.262 71.344	1.00 24.56 1.00 24.88 1.00 22.25 1.00 25.08
55	ATOM ATOM ATOM ATOM ATOM	7459 7460 7461 7462 7463	C GLU B 20 O GLU B 20 CB GLU B 20 CG GLU B 20 CD GLU B 20	6 62.268 6 63.314 6 62.523 6 62.593	78.488 78.744 77.961 76.964	72.381 72.938 69.973 68.847	1.00 26.18 1.00 27.62 1.00 29.23 1.00 26.21 1.00 27.07
60	ATOM ATOM ATOM ATOM	7464 7465 7466 7467	OE1 GLU B 200 OE2 GLU B 200 N VAL B 200 CA VAL B 200	6 64.470 6 63.914 7 61.188	76.004 75.143 79.198	68.948 69.936 68.037 72.641 73.586	1.00 27.64 1.00 28.80 1.00 25.55 1.00 27.27 1.00 27.65
65	ATOM ATOM ATOM ATOM ATOM	7468 7469 7470 7471 7472	C VAL B 20° O VAL B 20° CB VAL B 20° CG1 VAL B 20° CG2 VAL B 20°	7 60.983 7 61.803 7 60.525 7 60.995	79.914 80.149 81.538 82.724	75.030 75.933 73.137 73.892	1.00 26.94 1.00 25.85 1.00 28.03 1.00 27.28
70	ATOM ATOM ATOM ATOM	7473 7474 7475 7476	N PHE B 208 CA PHE B 208 C PHE B 208 O PHE B 208	59.836 59.503 59.844	79.306 79.017 77.614	71.645 75.281 76.672 77.116 78.298	1.00 27.49 1.00 26.63 1.00 26.90 1.00 26.57 1.00 25.78

	ATOM	7477	СВ	PHE	B	208		57.989	79.174	77.000	1.00 27.24
	ATOM	7478	CG	PHE		208		57.488	80.562	76.986	1.00 27.03
	ATOM	7479		PHE		208		58.328	81.623	76.747	1.00 28.32
	ATOM	7480	CD2	PHE	В	208		56.145	80.800	77.176	1.00 27.44
5	ATOM	7481	CE1	PHE	В	208		57.823	82.921	76.700	1.00 28.05
	ATOM	7482	CE2			208		55.633	82.068	77.118	1.00 28.17
	ATOM	7483	CZ	PHÉ		208	•	56.482	83.138	76.888	1.00 28.67
	ATOM	7484	N	SER		209		59.990	76.662	76.191	1.00 26.62
	ATOM	7485	CA	SER		209		60.105	75.245	76.577	1.00 26.13
10	ATOM	7486	C	SER		209		58.900	74.899	77.448	1.00 26.36
	ATOM	7487	0			209		58.979	74.171	78.431	1.00 26.32
	ATOM	7488	CB	SER SER		209		61.416 62.530	74.957 75.099	77.306 76.429	1.00 25.55 1.00 25.11
	ATOM ATOM	7489 7490	OG N	ALA				57.767	75.434	77.053	1.00 25.11
15	ATOM	7491	CA	ALA				56.530	75.139	77.750	1.00 20.03
13	ATOM	7492	C	ALA				55.368	75.586	76.863	1.00 26.75
	ATOM	7493	ŏ	ALA				55.554	76.453	75.977	1.00 26.11
	ATOM	7494	ČВ	ALA				56.496	75.835	79.162	1.00 26.29
	ATOM	7495	N	TYR		211		54.219	74.938	77.065	1.00 26.90
20	ATOM	7496	CA	TYR	В	211		52.957	75.218	76.366	1.00 27.97
	MOTA	7497	С	TYR	В	211		52.230	76.354	77.033	1.00 28.34
	ATOM	7498	0	TYR				51.469	77.130	76.423	1.00 27.52
	ATOM	7499	CB	TYR				52.034	74.021	76.525	1.00 28.35
	MOTA	7500	CG	TYR				50.822	74.005	75.605	1.00 28.82
25	ATOM	7501	CD1					50.772	74.750	74.417	1.00 28.38
	ATOM	7502	CD2	TYR				49.740	73.223	75.910	1.00 28.18
	ATOM	7503	CE1 CE2	TYR TYR				49.648 48.642	74.707 73.164	73.595 75.092	1.00 25.00 1.00 26.81
	ATOM ATOM	7504 7505	CEZ	TYR				48.594	73.104	73.092	1.00 24.68
30	ATOM	7506	OH	TYR				47.446	73.795	73.184	1.00 24.00
50	ATOM	7507	N	SER				52.473	76.413	78.330	1.00 29.04
	MOTA	7508	CA	SER				51.835	77.354	79.211	1.00 29.32
	ATOM	7509	C	SER		212		52.259	78.790	78.947	1.00 28.36
	ATOM	7510	0	SER				53.408	79.068	78.695	1.00 28.30
35	ATOM	7511	CB	SER	В	212		52.195	76.983	80.642	1.00 29.52
	ATOM	7512	OG	SER	В	212		51.407	77.736	81.521	1.00 34.46
	ATOM	7513	N	ALA				51.326	79.708	79.038	1.00 28.09
	MOTA	7514	CA	ALA				51.693	81.106	78.991	1.00 28.66
40	ATOM	7515	C	ALA				50.814	81.878	79.964	1.00 29.25
40	ATOM	7516	O	ALA				50.257	82.912	79.640	1.00 29.81
	ATOM ATOM	7517 7518	CB N	ALA LEU		213 214		51.579 50.728	81.627 81.325	77.605 81.162	1.00 28.39 1.00 30.34
	ATOM	7519	CA	LEU				49.974	81.843	82.308	1.00 30.34
	ATOM	7520	C	LEU				50.925	81.979	83.496	1.00 30.30
45	ATOM	7521	ŏ	LEU				51.700	81.089	83.752	1.00 29.34
	ATOM	7522	СB	LEU				48.948	80.788	82.727	1.00 31.14
	ATOM	7523	CG	LEU	В	214		47.513	80.885	82.229	1.00 33.58
	ATOM	7524	CD1	LEU	В	214		47.436	81.255	80.838	1.00 36.22
	ATOM	7525	CD2	LEU				46.847	79.558	82.415	1.00 34.93
50	MOTA	7526	N	TRP				50.872	83.070	84.228	1.00 30.57
	MOTA	7527	CA	TRP				51.706	83.193	85.419	1.00 30.30
	ATOM	7528	C	TRP				50.869	83.817	86.503	1.00 30.05
	ATOM	7529	O	TRP TRP				50.581	84.989 84.052	86.471	1.00 30.63 1.00 29.99
55	MOTA MOTA	7530 7531	CB CG	TRP				52.962 53.786	83.601	85.179 84.035	1.00 29.99
33	ATOM	7532		TRP				54.843	82.727	84.077	1.00 31.13
	ATOM	7532		TRP				53.608	83.950	82.649	1.00 29.56
	ATOM	7534	NE1					55.345	82.537	82.811	1.00 32.00
	ATOM	7535	CE2	TRP				54.600	83.257	81.913	1.00 31.76
60	ATOM	7536	CE3	TRP				52.714	84.779	81.960	1.00 26.48
_	ATOM	7537	CZ2	TRP				54.720	83.359	80.511	1.00 32.58
	ATOM	7538	CZ3	TRP	В	215		52.810	84.873	80.562	1.00 31.02
	ATOM	7539	CH2	TRP	В	215		53.820	84.172	79.854	1.00 32.58
	MOTA	7540	N	TRP				50.484	83.038	87.478	1.00 30.12
65	MOTA	7541	CA	TRP				49.760	83.593	88.609	1.00 30.31
	ATOM	7542	C	TRP				50.637	84.422	89.529	1.00 30.86
	ATOM	7543	0	TRP				51.828	84.183	89.634	1.00 31.61
	MOTA	7544	CB	TRP				49.214	82.478	89.461	1.00 29.58
70	ATOM	7545 7546	CG CD1	TRP				48.015 47.986	81.767 80.546	88.979 88.384	1.00 28.91 1.00 29.29
70	MOTA	/ 540	CDI	IKP	ם	210		-1.500	30.340	00.504	1.00 43.43

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_	ATOM ATOM ATOM ATOM	754 754 755	8 NE1 TRP B 216 9 CE2 TRP B 216 0 CE3 TRP B 216	46.646 82.147 89.184 1.00 28.16 46.688 80.168 88.161 1.00 31.36 45.845 81.133 88.638 1.00 28.27 46.016 83.268 89.742 1.00 29.24
5	ATOM ATOM ATOM ATOM	755 755: 755: 755:	2 CZ3 TRP B 216 3 CH2 TRP B 216	44.457 81.193 88.627 1.00 30.27 44.628 83.340 89.726 1.00 31.04 43.853 82.293 89.191 1.00 29.17 50.037 85.441 90.143 1.00 31.96
10	MOTA OTOM ATOM ATOM ATOM	755: 755: 755: 755:	5 CA SER B 217 6 C SER B 217 7 O SER B 217	50.629 86.205 91.257 1.00 32.49 50.974 85.256 92.383 1.00 32.33 50.307 84.243 92.544 1.00 30.55
15	MOTA MOTA MOTA MOTA	7559 7560 7562 7563	9 OG SER B 217 0 N PRO B 218 1 CA PRO B 218 2 C PRO B 218 3 O PRO B 218	49.459 88.290 91.440 1.00 34.18 51.911 85.632 93.244 1.00 33.78 52.202 84.814 94.428 1.00 34.88 51.001 84.778 95.355 1.00 36.39 50.806 83.758 95.986 1.00 37.96
20	ATOM ATOM ATOM ATOM ATOM ATOM	7564 7565 7566 7567 7568 7569	G CG PRO B 218 G CD PRO B 218 N ASN B 219 G CA ASN B 219	53.396 85.525 95.063 1.00 35.69 54.005 86.295 93.922 1.00 35.14 52.783 86.806 93.157 1.00 33.44 50.232 85.859 95.397 1.00 37.49 48.946 85.987 96.108 1.00 39.26
25	ATOM ATOM ATOM ATOM	7570 7571 7572 7573	O ASN B 219 CB ASN B 219 CG ASN B 219 OD1 ASN B 219	47.896 85.043 95.565 1.00 39.67 47.089 84.442 96.291 1.00 39.72 48.330 87.410 95.850 1.00 38.98 48.433 88.345 97.060 1.00 41.91 48.311 87.888 98.183 1.00 46.79
30	ATOM ATOM ATOM ATOM ATOM	7574 7575 7576 7577 7578	N GLY B 220 CA GLY B 220 C GLY B 220	48.625 89.664 96.831 1.00 40.99 47.865 84.980 94.246 1.00 39.21 46.757 84.360 93.561 1.00 38.69 45.819 85.466 93.098 1.00 38.39 44.786 85.208 92.488 1.00 38.87
35	ATOM ATOM ATOM ATOM ATOM	7579 7580 7581 7582 7583	N THR B 221	46.198 86.709 93.358 1.00 37.66 45.350 87.810 93.017 1.00 37.51 45.312 88.018 91.540 1.00 37.18 44.240 88.020 90.946 1.00 36.90
40	ATOM ATOM ATOM ATOM ATOM	7584 7585 7586 7587 7588	OG1 THR B 221 CG2 THR B 221 N PHE B 222 CA PHE B 222 C PHE B 222	45.452 89.073 95.067 1.00 39.62 45.083 90.325 93.187 1.00 37.99 46.495 88.197 90.954 1.00 36.74 46.612 88.519 89.558 1.00 36.26
45	ATOM ATOM ATOM ATOM ATOM	7589 7590 7591 7592 7593	O PHE B 222 CB PHE B 222 CG PHE B 222 CD1 PHE B 222 CD2 PHE B 222	47.702 86.467 89.069 1.00 36.16 47.740 89.503 89.318 1.00 35.78 47.521 90.848 89.914 1.00 37.68 46.630 91.752 89.335 1.00 37.31
50	ATOM ATOM ATOM ATOM ATOM	7594 7595 7596 7597 7598	CE1 PHE B 222 CE2 PHE B 222 CZ PHE B 222 N LEU B 223 CA LEU B 223	48.253 91.252 91.030 1.00 37.75 46.446 93.032 89.887 1.00 37.85 48.072 92.530 91.576 1.00 38.13 47.179 93.415 91.009 1.00 37.06 46.328 87.331 87.488 1.00 35.02 46.599 86.308 86.501 1.00 35.02
55	ATOM ATOM ATOM ATOM ATOM	7599 7600 7601 7602 7603	C LEU B 223 O LEU B 223 CB LEU B 223 CG LEU B 223 CD1 LEU B 223	47.239 87.009 85.291 1.00 33.64 46.591 87.766 84.585 1.00 34.11 45.301 85.598 86.101 1.00 34.43 45.364 84.124 85.650 1.00 37.73 44.380 83.825 84.519 1.00 35.89
60	ATOM ATOM ATOM ATOM ATOM	7604 7605 7606 7607 7608	CD2 LEU B 223 N ALA B 224 CA ALA B 224 C ALA B 224 O ALA B 224	46.763 83.670 85.228 1.00 37.28 48.524 86.815 85.068 1.00 32.28 49.121 87.381 83.858 1.00 31.54 49.196 86.324 82.780 1.00 30.26
65	ATOM ATOM ATOM ATOM ATOM	7609 7610 7611 7612 7613	CB ALA B 224 N TYR B 225 CA TYR B 225 C TYR B 225 O TYR B 225	50.481 87.937 84.122 1.00 31.38 49.154 86.766 81.522 1.00 30.30 49.173 85.882 80.367 1.00 29.65 49.641 86.597 79.120 1.00 29.29 49.570 87.822 78.998 1.00 29.09
70	ATOM ATOM ATOM	7614 7615 7616	CB TYR B 225 CG TYR B 225 CD1 TYR B 225	47.801 85.269 80.059 1.00 29.11 46.745 86.248 79.586 1.00 30.78 45.958 86.910 80.487 1.00 32.08

	ATOM ATOM	7617 7618	CD2 CE1	TYR	В	225 225	46.512 44.970	86.490 87.785	78.230 80.089	1.00	30.84 31.25
_	ATOM ATOM	7619 7620	CE2	TYR	В	225 225	45.530 44.767	87.377 88.025	77.835		32.45
5	ATOM ATOM	7621 7622	OH N			225 226	43.766 50.127	88.926 85.782	78.436 78.196		34.02 28.63
	ATOM	7623	CA	ALA ALA		226	50.610 49.622	86.237 85.793	76.907 75.854	1.00	
	ATOM ATOM	7624 7625	C O	ALA			49.622	84.793	76.027	1.00	
10	ATOM	7626	CB	ALA GLN			51.983 49.595	85.621 86.533	76.608 74.761		27.99 27.13
	ATOM ATOM	7627 7628	N CA	GLN			49.595	86.216	73.620		27.13
	ATOM	7629	C	GLN			49.612	86.226	72.383		27.32
15	ATOM ATOM	7630 7631	O CB	GLN GLN			50.416 47.664	87.141 87.257	72.181 73.452		25.90 28.61
	ATOM	7632	CG	GLN	В	227	46.691	86.956	72.370	1.00	27.98
	ATOM ATOM	7633 7634	CD OE1	GLN GLN		227 227	45.812 46.259	88.148 89.131	72.094 71.487		29.34 29.32
	ATOM	7635	NE2	GLN	В	227	44.579	88.086	72.559	1.00	25.03
20	ATOM	7636 7637	N CA	PHE PHE		228 228	49.498 50.315	85.179 85.107	71.583 70.405		26.63 27.20
	ATOM ATOM	7638	CA	PHE		228	49.429	85.135	69.209		26.71
	ATOM	7639	0	PHE		228	48.351	84.548	69.235		28.26
25	ATOM ATOM	7640 7641	CB CG	PHE PHE		228	51.194 51.989	83.894 83.746	70.415 71.681		26.80 27.53
	ATOM	7642		PHE	В	228	53.196	84.397	71.831		25.12
	ATOM	7643 7644	CD2 CE1			228 228	51.517 53.927	82.964 84.259	72.729 72.979		24.95 23.41
	ATOM ATOM	7645	CE2			228	52.264	82.821	73.888		24.50
30	ATOM	7646	CZ	PHE		228	53.472	83.460	74.006		22.75
	ATOM ATOM	7647 7648	N CA	ASN ASN		229 229	49.865 49.084	85.851 85.996	68.186 66.988		26.75 28.12
	MOTA	7649	С	ASN	В	229	49.925	85.496	65.821	1.00	28.58
35	ATOM ATOM	7650 7651	O CB	ASN ASN			50.984 48.654	86.052 87.465	65.514 66.821		28.66 28.28
<i>JJ</i>	ATOM	7652	CG	ASN	В	229	47.711	87.671	65.636		28.87
	ATOM ATOM	7653 7654		ASN ASN			47.694 46.909	86.887 88.711	64.668 65.731		27.69 32.77
	ATOM	7655	N N	ASP			49.438	84.422	65.198		29.23
40	ATOM	7656	CA	ASP			50.127	83.693	64.139		29.42
	ATOM ATOM	7657 7658	C O	ASP ASP			49.504 49.922	83.839 83.182	62.730 61.765		29.87 28.49
	MOTA	7659	СВ	ASP	В	230	50.094	82.215	64.530		29.90
45	ATOM ATOM	7660 7661	CG OD1	ASP ASP		230	51.209 51.273	81.847 82.457	65.465 66.540		30.77 36.25
	ATOM	7662		ASP	В	230	52.063	80.994	65.214	1.00	31.62
	ATOM ATOM	7663 7664	N CA	THR THR			48.533 47.829	84.724	62.620 61.365		30.50 31.25
	ATOM	7665	C	THR			48.641	84.879	60.118		31.98
50	ATOM	7666	0	THR			48.215	84.207	59.184		33.25
	ATOM ATOM	7667 7668	CB OG1	THR THR			47.149 46.132	86.272 86.231	61.366 62.345		31.46 31.85
	MOTA	7669	CG2	THR	В	231	46.333	86.506	60.005	1.00	34.71
55	ATOM ATOM	7670 7671	N CA	GLU GLU			49.772 50.509	85.569 85.533	60.046 58.801		31.14 31.74
<i>JJ</i>	ATOM	7672	C	GLU	В	232	51.747	84.650	58.894	1.00	30.99
	ATOM	7673	0	GLU GLU			52.658 50.931	84.822 86.941	58.132 58.413		30.42 33.19
	ATOM ATOM	7674 7675	CB CG	GLU			49.805	87.952	58.494		36.69
60	MOTA	7676	CD	GLU			50.150	89.268	57.821		43.55
	ATOM ATOM	7677 7678	-	GLU GLU			50.032 50.526	89.349 90.218	56.567 58.561		45.34 48.36
	MOTA	7679	N	VAL	В	233	51.805	83.752	59.872	1.00	29.36
65	ATOM ATOM	7680 7681	CA	VAL VAL			52.922 52.656	82.852 81.746	59.945 58.927		28.97 27.82
5 5	ATOM	7682	С О	VAL			51.558	81.243	58.860		27.82
	MOTA	7683	CB	VAL	В	233	53.056	82.322	61.344	1.00	29.57
	ATOM ATOM	7684 7685		VAL VAL			54.181 53.265	81.310 83.519	61.438 62.340		29.42 31.02
70	MOTA	7686	N	PRO			53.611	81.429	58.066		27.73

	ATOM	7687	CA	PRO B 23	4	53.378	80.375	57.063	1.00 28.03
	ATOM	7688		PRO B 23		53.297		57.693	
	ATOM			PRO B 23	4	53.815		58.790	
_	ATOM	7690		PRO B 23		54.580		56.115	
5		7691		PRO B 23		55.243		56.477	1.00 28.38
	ATOM	7692		PRO B 23		54.928		57.908	
	ATOM	7693		LEU B 23		52.607		57.008	
	ATOM ATOM	7694 7695		LEU B 23		52.366		57.502	
10		7695 7696		LEU B 23		53.280		56.922	1.00 27.09
10	ATOM	7697	O CB	LEU B 23 LEU B 23		53.567		55.734	
	ATOM	7698	CG	LEU B 23		50.918		57.165	1.00 29.04
	ATOM	7699		LEU B 23	_	49.888 48.532		57.648	1.00 30.71
	ATOM	7700	CD2	LEU B 23		49.669	77.339 77.245	56.918	1.00 34.01
15		7701	N	ILE B 23		53.806	74.853	59.095 57.781	1.00 30.08 1.00 25.72
	ATOM	7702	CA	ILE B 23		54.442	73.660	57.283	1.00 23.72
	ATOM	7703	С	ILE B 23		53.316	72.667	57.124	1.00 24.38
	ATOM	7704	0	ILE B 23	5	52.377	72.597	57.938	1.00 23.94
	ATOM	7705	CB	ILE B 23	5	55.598	73.143	58.182	1.00 25.42
20	MOTA	7706	CG1			56.360	72.041	57.439	1.00 28.92
	ATOM	7707	CG2		5	55.122	72.770	59.579	1.00 26.00
	ATOM	7708	CD1			56.567	70.833	58.283	1.00 33.95
	ATOM	7709	N	GLU B 23		53.410	71.894	56.069	1.00 23.99
25	ATOM	7710	CA	GLU B 23		52.372	70.939	55.679	1.00 24.82
25	ATOM ATOM	7711	C	GLU B 23		53.073	69.617	55.389	1.00 24.01
	ATOM	7712 7713	O	GLU B 23		54.087	69.604	54.769	1.00 23.08
	ATOM	7714	CB CG	GLU B 23'		51.611		54.459	1.00 24.84
	ATOM	7715	CD	GLU B 23		50.961 49.817	72.848	54.752	1.00 27.02
30	ATOM	7716	OE1	_		49.655	73.264 72.689	53.816	1.00 30.40
	ATOM	7717	OE2	GLU B 23		49.055	74.198	52.733 54.167	1.00 30.28
	ATOM	7718	N	TYR B 238		52.601	68.533	55.978	1.00 33.11 1.00 23.87
	ATOM	7719	CA	TYR B 238		53.143	67.213	55.721	1.00 23.87 1.00 23.57
	ATOM	7720	C	TYR B 238		52.022	66.237	55.926	1.00 24.22
35	ATOM	7721	0	TYR B 238		51.055	66.512	56.644	1.00 22.25
•	MOTA	7722	CB	TYR B 238		54.342	66.855	56.632	1.00 23.29
	ATOM	7723	CG	TYR B 238		54.099	67.003	58.135	1.00 24.82
	ATOM	7724	CD1	TYR B 238		54.357	68.200	58.773	1.00 24.60
40	ATOM	7725	CD2	TYR B 238		53.622	65.964	58.897	1.00 25.53
40	ATOM	7726	CE1	TYR B 238		54.136	68.368	60.097	1.00 25.40
	ATOM ATOM	7727	CE2	TYR B 238		53.413	66.126	60.293	1.00 24.43
	ATOM	7728 7729	CZ OH	TYR B 238		53.694	67.340	60.857	1.00 24.49
	ATOM	7730	N	SER B 239		53.549	67.600	62.182	1.00 25.79
45	ATOM	7731	CA	SER B 239		52.164 51.223	65.090	55.265	1.00 25.22
	ATOM	7732	C	SER B 239		51.349	63.983 63.189	55.363	1.00 25.50
	ATOM	7733	ŏ	SER B 239		52.422	63.109	56.649 57.174	1.00 25.41 1.00 26.57
	MOTA	7734	СB	SER B 239		51.485	63.044	54.211	1.00 26.37
	ATOM	7735	ŌG	SER B 239		51.186	63.705	53.021	1.00 23.24
50	ATOM	7736	N	PHE B 240		50.220	62.717	57.179	1.00 25.98
	ATOM	7737	CA	PHE B 240		50.158	61.814	58.320	1.00 25.45
	ATOM	7738	C	PHE B 240		49.294	60.655	57.830	1.00 25.82
	ATOM	7739		PHE B 240		48.155	60.873	57.414	1.00 25.70
	ATOM	7740		PHE B 240		49.484	62.466	59.537	1.00 25.55
55	ATOM	7741		PHE B 240		49.625	61.658	60.781	1.00 25.99
	ATOM	7742		PHE B 240		50.773	61.749	61.550	1.00 28.27
	ATOM	7743		PHE B 240		48.679	60.743	61.130	1.00 26.52
	ATOM	7744		PHE B 240		50.940	60.961	62.696	1.00 29.81
60	ATOM	7745		PHE B 240		48.852	59.949	62.251	1.00 28.54
00	ATOM ATOM	7746		PHE B 240		49.990	60.060	63.027	1.00 29.91
	ATOM	7747 7748		TYR B 241		49.820	59.437	57.868	1.00 25.66
	ATOM	7749		TYR B 241		49.142	58.310	57.264	1.00 25.52
	ATOM	7750		TYR B 241 TYR B 241		48.157	57.530	58.182	1.00 26.95
65	ATOM	7751		TYR B 241		47.129 50.208	57.045	57.706	1.00 25.02
55	ATOM	7752		TYR B 241		50.208	57.419	56.620	1.00 25.51
	ATOM	7753		TYR B 241		50.642	58.205 58.430	55.630	1.00 25.02
	ATOM	7754		TYR B 241		52.313	58.430 58.742	54.333 56.019	1.00 24.85
	ATOM	7755		TYR B 241		51.385	59.183	53.434	1.00 24.74 1.00 24.84
70	ATOM	7756		TYR B 241		53.084	59.469	55.143	1.00 24.84
									1.00 23.24

	ATOM	7757	CZ	TYR			52.599	59.681	53.841		24.72
	ATOM	7758	ОН	TYR			53.307	60.384	52.982		25.39
	ATOM	7759	N	SER SER			48.442 47.718	57.507 56.743	59.498 60.527		28.06 28.10
5	ATOM ATOM	7760 7761	CA C	SER		242	47.718	55.270	60.275	_	27.38
3	ATOM	7762	ŏ	SER		242	48.408	54.696	59.581		27.05
	ATOM	7763	ČВ	SER	_	242	46.339	57.314	60.912		28.67
	ATOM	7764	OG	SER	В	242	45.832	58.068	59.883		34.27
	ATOM	7765	N	ASP			46.621	54.657	60.943		27.89
10	MOTA	7766	CA	ASP			46.342	53.244	60.845		29.32
	ATOM	7767	C	ASP		243	46.001	52.909	59.380		28.89 29.54
	ATOM ATOM	7768 7769	O CB	ASP ASP		243	45.590 45.185	53.790 52.876	58.607 61.818		30.16
	ATOM	7770	CG	ASP		243	45.456	53.350	63.300		35.73
15	ATOM	7771		ASP			46.600	53.169	63.810		38.58
•	ATOM	7772	OD2				44.608	53.961	64.025		39.36
	ATOM	7773	N	GLU	В	244	46.212	51.669	58.987	1.00	28.75
	ATOM	7774	CA	GLU			45.862	51.205	57.648		30.00
••	ATOM	7775	C	GLU			44.417	51.504	57.191		29.87
20	ATOM	7776	0	GLU GLU		244	44.161 45.847	51.540 49.685	55.985 57.590		29.78 31.02
	ATOM ATOM	7777 7778	CB CG	GLU			47.091	49.003	57.831		33.19
	ATOM	7779	CD	GLU		244	46.840	47.448	57.551		37.41
	ATOM	7780		GLU			46.089	47.131	56.597		35.31
25	ATOM	7781	OE2				47.418	46.600	58.279	1.00	43.04
	ATOM	7782	N	SER			43.478	51.638	58.136		28.42
	MOTA	7783	CA	SER			42.078	51.855	57.793		28.88
	ATOM	7784	Č	SER			41.792	53.213	57.185		27.78
20	ATOM	7785 7786	O CB	SER SER		245 245	40.774 41.185	53.415 51.664	56.553 59.043		29.01 28.82
30	ATOM ATOM	7787	OG	SER			41.671	52.500	60.086		30.11
	ATOM	7788	Ŋ	LEU			42.658	54.173	57.389		26.88
	ATOM	7789	CA	LEU		246	42.419	55.476	56.821	1.00	27.33
	ATOM	7790	С	LEU		246	42.697	55.448	55.306		26.18
35	ATOM	7791	0	LEU		246	43.813	55.191	54.876	1.00	
	ATOM	7792	CB	LEU		246	43.354	56.483	57.425		27.45
	ATOM	7793 7794	CG CD1	LEU LEU		246	42.894 43.988	57.878 58.847	57.761 57.373		31.22 32.53
	ATOM ATOM	7795		LEU			41.541	58.313	57.252		31.50
40	ATOM	7796	N	GLN			41.701	55.804	54.528	1.00	
	ATOM	7797	CA	GLN		247	41.773	55.696	53.090	1.00	25.50
	MOTA	7798	С	GLN		247	42.559	56.842	52.452		25.73
	MOTA	7799	0	GLN		247	43.349	56.623	51.553		26.11
45	ATOM	7800	CB	GLN			40.339	55.580	52.521	1.00	24.84 25.22
4 5	ATOM ATOM	7801 7802	CG CD	GLN GLN			40.311 38.897	55.160 54.968	51.065 50.524		25.36
	ATOM	7802	_	GLN			37.963	55.646	50.962	1.00	
	ATOM	7804		GLN			38.741	54.041	49.583		21.11
	MOTA	7805	Ν.	TYR	В	248	42.307	58.063	52.886	1.00	26.15
50	MOTA	7806	CA	TYR			43.064	59.198	52.417		26.69
	ATOM	7807	C	TYR			43.936	59.730	53.539		27.73
	MOTA	7808	0	TYR			43.465	59.967	54.649 51.953		27.01 26.34
	ATOM ATOM	7809 7810	CB CG	TYR TYR			42.149 41.422	60.327 60.005	50.663		27.01
55	ATOM	7811		TYR			40.307	59.173	50.666		26.91
55	ATOM	7812		TYR			41.840	60.546	49.441		27.29
	ATOM	7813		TYR			39.604	58.896	49.493		27.29
	MOTA	7814	CE2				41.154	60.242	48.248		28.74
	MOTA	7815	CZ	TYR			40.044	59.408	48.291		27.43
60	MOTA	7816	OH	TYR			39.357	59.124	47.142 53.242		24.10 28.25
	ATOM ATOM	7817 7818	N CA	PRO PRO			45.213 46.134	59.930 60.497	54.223		28.79
	ATOM	7819	CA	PRO			45.698	61.885	54.691		29.17
	ATOM	7820	Ö	PRO			45.064	62.633	53.951		26.49
65	ATOM	7821	ČВ	PRO			47.462	60.574	53.462		28.57
	MOTA	7822	CG	PRO			47.306	59.622	52.325		29.61
	MOTA	7823	CD	PRO			45.876	59.583	51.984		27.88
	ATOM	7824	N	LYS			45.985	62.191	55.961		29.80
70	ATOM	7825	CA	LYS			45.693	63.513	56.475		29.97
70	MOTA	7826	С	LYS	Ħ	∠⊃U	46.885	64.417	56.200	1.00	29.32

	ATOM ATOM ATOM	7827 7828 7829	CB CG	LYS	B 250 B 250 B 250	48.024 45.389 44.694	63.469	57.988	1.00 31.46
5	ATOM ATOM ATOM ATOM	7830 7831 7832 7833	CE NZ	LYS LYS	B 250 B 250 B 250 B 251	44.889 45.094 45.086 46.601	65.052 66.583 66.930	60.033 60.300 61.773 56.025	1.00 41.42 1.00 43.24 1.00 45.60 1.00 28.46
10	ATOM ATOM ATOM ATOM	7834 7835 7836 7837		THR THR	B 251 B 251 B 251 B 251	47.616 47.671 46.720 47.323	66.698 67.550 68.218	55.877 57.163 57.493 54.675	1.00 28.16 1.00 27.00 1.00 27.97 1.00 28.23
15	ATOM ATOM ATOM ATOM	7838 7839 7840 7841	OG1 CG2 N CA	VAL VAL	B 251 B 252 B 252	47.486 48.390 48.786 48.999	66.860 68.676 67.493	53.467 54.558 57.873 59.078	1.00 27.70 1.00 28.77 1.00 25.71 1.00 25.09
	ATOM ATOM ATOM ATOM	7842 7843 7844 7845	C O CB CG1	VAL	B 252 B 252 B 252 B 252	49.496 50.368 50.022 50.202	69.653 69.785 67.564	58.664 57.804 59.975 61.320	1.00 25.01 1.00 23.34 1.00 25.60 1.00 25.24
20	ATOM ATOM ATOM ATOM	7846 7847 7848 7849	CG2 N CA C	ARG :	B 252 B 253 B 253 B 253	49.564 48.889 49.261 49.566	66.168 70.684 72.040	60.247 59.224 58.915 60.236	1.00 26.76 1.00 24.91 1.00 26.21 1.00 25.85
25	ATOM ATOM ATOM ATOM	7850 7851 7852 7853	O CB CG CD	ARG I	B 253	48.699 48.141 47.931 46.673	72.761	61.087 58.151 56.759 56.041	1.00 26.18 1.00 26.65 1.00 31.04 1.00 36.68
30	ATOM ATOM ATOM ATOM ATOM	7854 7855 7856 7857 7858	NE CZ NH1 NH2 N	ARG I ARG I ARG I VAL I	3 253 3 253 3 253	45.671 45.255 45.699 44.366 50.808	70.954	56.094 55.056 53.804 55.287	1.00 45.06 1.00 48.15 1.00 47.19 1.00 48.13
35	ATOM ATOM ATOM ATOM	7859 7860 7861 7862	CA C O CB	VAL I VAL I VAL I	3 254 3 254 3 254	51.248 51.866 52.764 52.329	73.868 75.230 75.357 73.064	60.400 61.599 61.307 60.500 62.258	1.00 25.30 1.00 25.01 1.00 25.27 1.00 24.30 1.00 24.74
40	ATOM ATOM ATOM ATOM ATOM	7863 7864 7865 7866 7867	CG1 CG2 N CA C	VAL E VAL E PRO E PRO E	3 254 3 255 3 255	52.731 51.902 51.413 52.028 53.450	73.675 71.651 76.257 77.582 77.486	63'.653 62.386 61.990 61.825 62.374	1.00 26.20 1.00 24.36 1.00 25.74 1.00 26.05 1.00 26.44
45	ATOM ATOM ATOM	7868 7869 7870 7871	O CB CG CD	PRO E PRO E PRO E	3 255 3 255 3 255 3 255	53.583 51.156 49.849 50.316	77.224 78.486 77.683 76.248	63.562 62.661 62.869 62.959	1.00 25.74 1.00 26.77 1.00 27.04 1.00 26.03
50	ATOM ATOM ATOM	7872 7873 7874 7875	N CA C	TYR E TYR E TYR E	256 256 256 256	54.467 55.881 56.741 56.866	77.610 77.432 78.390 78.242	61.506 61.864 61.070 59.847	1.00 25.43 1.00 23.71 1.00 23.86 1.00 23.06
50	ATOM ATOM ATOM ATOM ATOM	7876 7877 7878 7879 7880	CB CG CD1 CD2 CE1	TYR E TYR E TYR E	256 256 256	56.275 57.692 58.773 57.929	76.019 75.536 76.045 74.518	61.451 61.692 60.985 62.579	1.00 24.30 1.00 23.12 1.00 23.72 1.00 22.68
55	ATOM ATOM ATOM ATOM	7881 7882 7883 7884	CE2 CZ OH N	TYR B TYR B TYR B TYR B PRO B	256 256 256	60.066 59.194 60.262 61.499	75.552 74.015 74.531 74.011	61.179 62.786 62.088 62.310	1.00 22.28 1.00 24.55 1.00 25.38 1.00 22.59
60	ATOM ATOM ATOM ATOM	7885 7886 7887 7888	CA C O CB	PRO B PRO B PRO B PRO B	257 257 257	57.347 58.211 59.554 60.275 58.429	79.378 80.350 79.785 79.547 81.473	61.732 61.038 60.746 61.674 62.068	1.00 23.65 1.00 23.40 1.00 22.75 1.00 24.71
65	ATOM ATOM ATOM ATOM	7889 7890 7891 7892	CG CD N CA	PRO B PRO B LYS B LYS B	257 257 258 258	58.042 57.282 59.874 61.198	80.886 79.604 79.580 79.199	63.474 63.181 59.491 59.030	1.00 24.29 1.00 24.80 1.00 24.55 1.00 23.80 1.00 23.19
70	ATOM ATOM ATOM ATOM	7893 7894 7895 7896	O CB	LYS B LYS B LYS B LYS B	258 258	62.111 61.674 61.108 60.637	80.462 81.591 78.534 77.040	59.053 59.259 57.642 57.673	1.00 24.02 1.00 20.36 1.00 23.36 1.00 22.40

	ATOM ATOM ATOM	7897 7898 7899	CD CE NZ	LYS E LYS E LYS E	258	60.277 59.820 60.874	76.473 74.992	56.281 56.340	1.00 23.16 1.00 22.40
	ATOM	7900	N	ALA B		63.407	74.018 80.229	56.757 58.956	1.00 21.29 1.00 26.33
5	ATOM	7901	CA	ALA B	259	64.377	81.292	59.168	1.00 27.36
	ATOM ATOM	7902 7903	C	ALA B		64.066 63.938	82.392 82.139	58.213 57.022	1.00 28.09 1.00 27.41
	ATOM	7904	СВ	ALA B		65.812	80.758	58.966	1.00 27.41
	ATOM	7905	N	GLY B	260	63.868	83.602	58.749	1.00 28.60
10	ATOM ATOM	7906 7907	CA C	GLY B		63.602 62.147	84.769	57.932	1.00 28.14 1.00 28.41
	ATOM	7908	Ö	GLY B		61.799	85.007 86.031	57.621 57.026	1.00 28.41
	ATOM	7909	N	ALA B	261	61.280	84.100	58.039	1.00 27.69
15	MOTA	7910 7911	CA	ALA B		59.862	84.234	57.713	1.00 28.41
13	ATOM ATOM	7911	C O	ALA B		59.130 59.684	85.087 85.417	58.742 59.797	1.00 27.69 1.00 26.36
	ATOM	7913	CB	ALA B	261	59.209	82.853	57.611	1.00 29.03
	ATOM	7914	N	VAL B		57.892	85.463	58.424	1.00 26.40
20	ATOM ATOM	7915 7916	CA C	VAL B		57.100 56.942	86.220 85.380	59.364 60.658	1.00 26.14 1.00 26.40
20	ATOM	7917	ŏ	VAL B		56.500	84.251	60.592	1.00 25.67
	ATOM	7918	CB	VAL B		55.689	86.556	58.816	1.00 26.61
	ATOM ATOM	7919 7920	CG1	VAL B		54.787 55.718	87.059 87.604	59.912 57.635	1.00 26.64 1.00 27.06
25	ATOM	7921	N	ASN B		57.300	85.950	61.815	1.00 25.81
	ATOM	7922	CA	ASN B		57.142	85.313	63.115	1.00 26.49
	ATOM ATOM	7923 7924	C	ASN B		55.807 55.209	85.708 86.670	63.721 63.280	1.00 25.87 1.00 26.72
	ATOM	7925	СB	ASN B		58.196	85.859	64.083	1.00 26.60
30	ATOM	7926	CG	ASN B		59.444	85.013	64.177	1.00 27.28
	ATOM ATOM	7927 7928		ASN B		60.455 59.415	85.469 83.804	64.758 63.640	1.00 33.18 1.00 18.52
	ATOM	7929	N	PRO B		55.324	84.997	64.732	1.00 18.32
	ATOM	7930	CA	PRO B	264	54.143	85.442	65.463	1.00 25.63
35	ATOM ATOM	7931 7932	C	PRO B		54.432	86.709	66.282	1.00 26.29
	ATOM	7933	O CB	PRO B		55.572 53.940	86.954 84.314	66.662 66.460	1.00 25.52 1.00 26.54
	ATOM	7934	CG	PRO B	264	55.338	83.804	66.699	1.00 24.95
40	ATOM ATOM	7935 7936	CD	PRO B	264 265	55.846 53.424	83.738	65.286	1.00 25.96
40	ATOM	7937	N CA	THR B		53.424	87.516 88.650	66.550 67.431	1.00 26.67 1.00 27.04
	ATOM	7938	C	THR B	265	53.054	88.264	68.773	1.00 26.93
	ATOM ATOM	7939 7940	O CB	THR B	-	52.300	87.304	68.888	1.00 24.94
45	ATOM	7941		THR B		52.860 51.525	89.840 89.412	66.942 66.683	1.00 27.26 1.00 25.84
	ATOM	7942	CG2	THR B	265	53.422	90.368	65.611	1.00 28.09
	ATOM ATOM	7943 7944	N CA	VAL B		53.357 52.907	89.073	69.779	1.00 27.81
	ATOM	7945	CA	VAL B		52.476	88.766 89.967	71.137 71.903	1.00 28.12 1.00 27.91
50	ATOM	7946	Ō	VAL B	266	52.986	91.042	71.695	1.00 28.76
	ATOM	7947	CB	VAL B		54.032	88.068	71.923	1.00 28.38
	ATOM ATOM	7948 7949		VAL B		55.318 53.630	88.852 87.871	71.856 73.366	1.00 30.25 1.00 29.69
	ATOM	7950	N	LYS B	267	51.524	89.769	72.808	1.00 28.94
55	MOTA	7951	CA	LYS B		50.987	90.823	73.663	1.00 29.03
	ATOM ATOM	7952 7953	C O	LYS B		50.978 50.955	90.238 89.011	75.054 75.206	1.00 28.26 1.00 26.79
	ATOM	7954	ČВ	LYS B	267	49.556	91.216	73.258	1.00 29.74
60	ATOM	7955	CG	LYS B		49.404	92.074	71.966	1.00 34.60
60	ATOM ATOM	7956 7957	CD CE	LYS B		50.108 49.430	93.458 94.624	72.157 71.317	1.00 40.68 1.00 44.72
	ATOM	7958	NZ	LYS B		49.882	96.041	71.682	1.00 42.65
	ATOM	7959	N	PHE B	268	51.020	91.112	76.060	1.00 28.28
65	ATOM ATOM	7960 7961	CA C	PHE B		51.060 50.017	90.697 91.429	77.453	1.00 28.24
0,5	ATOM	7962	0	PHE B		49.842	92.624	78.247 78.075	1.00 28.18 1.00 28.10
	ATOM	7963	СВ	PHE B	268	52.466	90.919	78.041	1.00 28.72
	ATOM	7964	CG	PHE B		52.652	90.334	79.425	1.00 27.25
70	MOTA MOTA	7965 7966		PHE B		53.019 52.450	89.030 91.100	79.583 80.539	1.00 26.79 1.00 28.85
- •						55.450			2.00 20.00

	ATOM	7967	7 CE	1 PHE	B 268	53	.180	88.488	80.803	1.00 26.99
	ATOM ATOM				B 268 B 268	52	.635	90.579	81.789	1.00 28.72
_	ATOM	7970) N	PHE	B 269		.991 .342	89.250 90.707		
5	ATOM ATOM				B 269 B 269		.229	91.238	79.890	1.00 29.07
	ATOM	7973	ō		B 269		.189 .738	90.753 89.698	81.329 81.678	
	MOTA MOTA	7974 7975			B 269 B 269		.912	90.772	79.266	1.00 29.33
10		7976		1 PHE			.636 .060	91.318 92.573	77.884 77.703	
	ATOM ATOM	7977 7978			B 269 B 269	46	.901	90.555	76.770	1.00 27.28
	ATOM	7979					.751 .617	93.025 91.011	76.404 75.522	1.00 31.90 1.00 27.59
15	ATOM ATOM	7980 7981			B 269	46	.041	92.249	75.338	1.00 29.73
13	ATOM	7982		VAL VAL			.467 .295	91.491 91.070	82.166 83.544	1.00 31.12 1.00 32.19
	ATOM	7983		VAL	В 270	45.	.900	91.401	83.950	1.00 32.90
	ATOM ATOM	7984 7985		VAL VAL			. 427 . 222	92.487 91.816	83.686 84.463	1.00 32.40 1.00 32.52
20		7986	CG1	VAL .	B 270	48.	212	91.172	85.864	1.00 32.32
	ATOM ATOM	- 7987 7988	N CG2	VAL :	B 270 B 271		631 259	91.835 90.453	83.863 84.604	1.00 32.85 1.00 33.75
	ATOM	7989	CA	VAL 1	B 271	43.	900	90.604	85.044	1.00 33.75
25	ATOM ATOM	7990 7991	С 0		B 271 B 271		826 457	90.377 89.457	86.539 87.045	1.00 35.04
	ATOM	7992	СВ	VAL	3 271	43.	025	89.491	84.457	1.00 33.68 1.00 35.21
	ATOM ATOM	7993 7994	CG1	VAL I	3 271 3 271		595 153	89.679 89.438	84.869	1.00 35.84
20	ATOM	7995	N	ASN I	3 272	43.	011	91.177	82.966 87.217	1.00 37.46 1.00 36.31
30	ATOM ATOM	7996 7997	CA C	ASN I			713 664	90.975 89.919	88.646	1.00 37.31
	MOTA	7998	0	ASN E	3 272	40.		90.091	88.809 88.427	1.00 37.75 1.00 37.06
	ATOM ATOM	7999 8000	CB CG	ASN E		42. 42.	178	92.246 92.185	89.300	1.00 38.06
35	MOTA	8001	OD1	ASN E	3 272	41.	886	91.172	90.817 91.434	1.00 37.62 1.00 37.86
	ATOM ATOM	8002 8003	ND2 N	ASN E		42. 42.		93.254	91.417	1.00 35.80
	MOTA	8004	CA	THR E	273	41.		88.842 87.665	89.452 89.632	1.00 39.53 1.00 40.60
40	ATOM ATOM	8005 8006	C O	THR E		40. 39.		87.769 86.948	90.834	1.00 42.89
	ATOM	8007	CB	THR E	273	42.		86.518	90.999 89.758	1.00 41.51 1.00 40.45
	ATOM ATOM	8008 8009	OG1 CG2	THR E		42. 42.		85.649	88.612	1.00 43.84
	MOTA	8010	N	ASP B	274	40.		85.673 88.789	90.930 91.661	1.00 38.99 1.00 45.49
45	ATOM ATOM	8011 8012	CA C	ASP B		39.		88.935	92.889	1.00 48.12
	ATOM	8013	0	ASP B	274	38.4 37.4		89.759 89.750	92.620 93.406	1.00 49.85 1.00 49.50
	ATOM ATOM	8014 8015	CB CG	ASP B		40.		89.570	94.003	1.00 48.46
50	ATOM	8016	OD1	ASP B	274	41.5 41.2		88.578 87.349	94.648 94.604	1.00 49.63 1.00 47.99
	ATOM ATOM	8017 8018	OD2 N	ASP B SER B		42.5	543	88.951	95.240	1.00 52.84
	ATOM	8019	CA	SER B		38.4 37.2		90.433 91.222	91.472 91.063	1.00 51.84 1.00 52.96
55	ATOM ATOM	8020 8021	C O	SER B		36.6	599	90.683	89.775	1.00 54.06
55	ATOM	8021	CB	SER B SER B		36.9 37.7		91.222 92.661	88.705 90.817	1.00 55.29 1.00 53.02
	ATOM ATOM	8023	OG	SER B	275	38.5	518	92.734	89.656	1.00 52.54
	ATOM	8024 8025	N CA	LEU B		35.9 35.3		89.623 89.070	89.852 88.649	1.00 54.49 1.00 54.65
60	ATOM	8026	C	LEU B	276	33.8	324	88.957	88.839	1.00 54.05
	ATOM ATOM	8027 8028		LEU B		33.3 35.9		88.767 87.707	89.945	1.00 54.57
	ATOM	8029	CG	LEU B	276	37.3	64	87.736	88.312 87.872	1.00 54.66 1.00 53.89
65	ATOM ATOM	8030 8031	CD1 CD2	LEU B LEU B	276 276	37.8 37.5		86.324 88.496	87.751	1.00 54.37
-	ATOM	8032	N	SER B	277	33.0	87	89.068	86.575 87.741	1.00 51.77 1.00 55.99
	ATOM ATOM	8033 8034		SER B		31.6 30.9		89.074	87.782	1.00 56.29
	ATOM	8035	0	SER B	277	31.3	82 8	87.959 87.717	86.971 85.826	1.00 56.82 1.00 56.20
70	ATOM	8036	СВ	SER B	277	31.1	14 9	90.397	87.257	1.00 56.23

	ATOM ATOM	8037 8038	OG N	SER SER	B 278	29.747 29.994	87.327	86.932 87.569	1.00 56.57 1.00 57.97
	ATOM	8039	CA	SER		29.334		86.985	1.00 58.95
-	MOTA	8040	Č	SER		28.986	86.391	85.543	1.00 59.89
5	ATOM	8041	0	SER I		29.183	85.492	84.726	1.00 60.37
	ATOM	8042	CB	SER I		28.078	85.777	87.775	1.00 59.11
	ATOM	8043	OG	SER I		28.378	84.786	88.768	1.00 59.81
	ATOM	8044	N	VAL		28.496	87.583	85.210	1.00 60.61
10	ATOM	8045	CA	VAL		28.110	87.840	83.829	1.00 61.05
10	ATOM	8046	C	VAL		28.938	88.901	83.086	1.00 60.36
	ATOM	8047	0	VAL		29.131	88.783	81.869	1.00 61.06
	ATOM	8048	CB	VAL		26.623	88,223	83.723	1.00 61.89
	ATOM	8049	CG1			26.075	87.713	82.398	1.00 63.23
1.5	ATOM	8050	CG2			25.816	87.640	84.889	1.00 62.56
15	ATOM	8051	N	THR I		29.422	89.920	83.800	1.00 59.14
	ATOM	8052	CA	THR I		30.189	91.037	83.197	1.00 57.83
	ATOM	8053	C	THR I		31.635	90.680	82.805	1.00 56.12
	ATOM	8054	0	THR I		32.362	90.043	83.576	1.00 56.22
20	ATOM	8055	CB	THR I		30.174	92.238	84.170	1.00 58.21
20	ATOM	8056	OG1			28.829	92.709	84.301	1.00 57.77
	ATOM	8057	CG2			30.957	93.466	83.618	1.00 58.84
	ATOM	8058	N	ASN I		32.039	91.121	81.613	1.00 54.01
	ATOM	8059	CA	ASN I		33.341	90.780	81.024	1.00 52.59
25	ATOM	8060	C	ASN I		34.552	91.311	81.799	1.00 51.17
25	ATOM	8061	0	ASN I	-	34.623	92.490	82.136	1.00 51.36
	ATOM	8062	CB	ASN I		33.381	91.205	79.543	1.00 52.22
	ATOM	8063	CG	ASN I		32.565	90.259	78.649	1.00 53.14
	MOTA	8064		ASN E		32.162	89.177	79.103	1.00 51.75
30	ATOM	8065		ASN E		32.329	90.646	77.377	1.00 50.81
30	ATOM ATOM	8066 8067	N CA	ALA E		35.495	90.416 90.743	82.083	1.00 49.39
	ATOM	8068	CA	ALA E		36.697	91.717	82.859 82.128	1.00 48.04
	ATOM	8069	0	ALA E		37.609 37.724			1.00 46.65
	ATOM	8070	СВ	ALA E		37.459	91.654 89.473	80.906 83.164	1.00 45.49 1.00 48.05
35	ATOM	8071	N	THR E		38.272	92.609	82.858	1.00 45.32
33	ATOM	8072	CA	THR E		39.188	93.534	82.193	1.00 45.32
	ATOM	8072	CA	THR E		40.644	93.048	82.252	1.00 43.17
	ATOM	8074	Ö	THR E		41.140	92.684	83.304	1.00 45.06
	ATOM	8075	СВ	THR E		39.093	94.945	82.806	1.00 45.56
40	ATOM	8076	OG1	THR E		37.791	95.509	82.557	1.00 47.54
10	ATOM	8077	CG2	THR E		40.033	95.895	82.089	1.00 45.76
	ATOM	8078	N	SER E		41.311	93.030	81.117	1.00 41.77
	ATOM	8079	CA	SER E		42.708	92.665	81.049	1.00 40.86
	ATOM	8080	C	SER E		43.529	93.929	80.874	1.00 39.75
45	ATOM	8081	ŏ	SER E		43.259	94.700	79.963	1.00 39.36
	ATOM	8082	CB	SER E		42.952	91.755	79.838	1.00 40.93
	ATOM	8083	ŌĞ	SER E		42.604	90.405	80.107	1.00 40.28
	ATOM	8084	N	ILE E		44.508	94.182		1.00 38.45
	ATOM	8085	CA	ILE E		45.354	95.348	81.495	1.00 37.90
50	ATOM	8086	С	ILE E		46.556	94.957	80.677	1.00 36.75
	ATOM	8087	0	ILE E		47.196	93.952	80.958	1.00 36.40
	ATOM	8088	CB	ILE E	285	45.752	96.057	82.781	1.00 37.70
	ATOM	8089	CG1	ILE E		44.512	96.661	83.435	1.00 39.24
	ATOM	8090	CG2	ILE E	285	46.701	97.209	82.477	1.00 37.80
55	ATOM	8091	CD1	ILE E	285	44.009	95.843	84.572	1.00 40.83
	ATOM	8092	N	GLN E	286	46.848	95.739	79.639	1.00 36.28
	ATOM	8093	CA	GLN E	286	47.933	95.408	78.741	1.00 36.02
	ATOM	8094	С	GLN E	286	49.270	96.017	79.167	1.00 36.44
	ATOM	8095	0	GLN B	286	49.335	97.183	79.507	1.00 35.96
60	ATOM	8096	CB	GLN B	286	47.611	95.830	77.294	1.00 35.59
	ATOM	8097	CG	GLN E	286	48.760	95.542	76.284	1.00 34.01
	ATOM	8098	CD	GLN B	286	48.368	95.650	74.794	1.00 30.38
	ATOM	8099	OE1	GLN B	286	47.325	96.170	74.437	1.00 32.82
	MOTA	8100	NE2	GLN B		49.197	95.133	73.951	1.00 27.98
65	MOTA	8101	N	ILE B		50.341	95.226	79.162	1.00 36.19
	MOTA	8102	CA	ILE B		51.628	95.820	79.365	1.00 36.28
	MOTA	8103	С	ILE B	287	52.345	95.765	78.029	1.00 36.85
	MOTA	8104	0	ILE B		52.539	94.720	77.428	1.00 36.85
_	MOTA	8105	CB	ILE B		52.455	95.182	80.477	1.00 36.53
70	MOTA	8106	CG1	ILE B	287	51.718	95.200	81.808	1.00 36.38

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MOTA
               8107
                      CG2 ILE B 287
                                             53.784
                                                      95.966
                                                                80.636
                                                                         1.00 36.09
       ATOM
               8108
                      CD1
                           ILE
                               В
                                  287
                                             52.495
                                                      94.510
                                                                82.943
                                                                         1.00 37.45
       ATOM
               8109
                      N
                           THR
                               B 288
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       ATOM
               8110
                      CA
                           THR
                               B 288
                                             53.355
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                                                               76.274
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                           THR B 288
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       ATOM
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75.753
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                           THR B
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                                                                         1.00 39.54
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                           ALA B 289
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      MOTA
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97.593
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      ATOM
                           PRO B 290
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                          PRO B 290
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                          PRO B 290
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59.780 101.186
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63.264
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      ATOM
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                          SER B 292
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              8136
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      ATOM
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                          SER B
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                          SER B 292
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              8140
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96.774
96.103
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70.041
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                                                                        1.00 37.42
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                                                     95.562
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93.932
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                     CG
                          MET
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     ATOM
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                          MET B 293
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                                                              72.473
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     ATOM
              8146
                    CE
                          MET B 293
                                           64.400
                                                     94.091
                                                              73.586
                                                                        1.00 36.67
     ATOM
              8147
                          LEU B 294
                    N
                                           59.524
                                                    97.705
                                                              70.268
                                                                        1.00 38.14
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                    CA
                                                    97.958
                                                              69.305
                                                                        1.00 38.99
     ATOM
              8149
                    С
                         LEU B 294
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98.590
                                                              67.991
66.995
                                           59.023
                                                                        1.00 39.37
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                    0
                                           58.341
                         LEU B 294
                                                                        1.00 39.80
1.00 39.18
45
     MOTA
             8151
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56.705
55.889
                    CB
                         LEU B 294
                                                    98.903
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     ATOM
             8152
                    CG
                         LEU
                             B 294
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                                                                        1.00 41.58
     ATOM
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                                                    99.401
97.135
                                                              71.811
                    CD1
                         LEU
                              В
                                294
                                                                        1.00 40.69
     MOTA
             8154
                    CD2
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                         LEU
                                                                        1.00 41.80
     ATOM
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                    N
                         ILE
                             B 295
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                                                              68.034
                                                                        1.00 39.37
50
     ATOM
             8156
                    CA
                                           61.001
60.918
                         ILE
                              B 295
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                                                              66.872
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             8157
     ATOM
                                                              65.744
64.579
67.359
                                                    98.331
98.695
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                         ILE
                              В
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     ATOM
             8158
                                           60.846
                    0
                         ILE B 295
                                                                       1.00 38.34
     MOTA
             8159
                    CB
                         ILE B 295
                                           62.441
                                                    99.617
                                                                       1.00 40.97
     ATOM
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                    CG1
                         ILE
                             B 295
                                           63.505
                                                    99.653
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     ATOM
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                    CG2
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66.952
                         ILE
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                                           62.868
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                    CD1
                         ILE B 295
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                    N
                         GLY B 296
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                                                              66.097
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             8164
                    CA
                         GLY B 296
                                           60.843
                                                    95.967
                                                              65.105
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    ATOM
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59.589
                    С
                         GLY B 296
                                                    94.616
                                                              65.635
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60
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                         GLY B 296
                                                             66.582
65.013
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    ATOM
             8167
                    N
                         ASP B 297
                                           60.779
                                                    93.521
                                                                       1.00
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    MOTA
             8168
                    CA
                         ASP
                             B 297
                                           60.367
                                                    92.200
                                                             65.458
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                         ASP
                             В
                                297
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                                                    91.884
                                                             66.815
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    ATOM
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                    0
                         ASP
                             В
                                297
                                           62.251
                                                    92.111
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                    CB
                         ASP B
                               297
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                                                                       1.00
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    MOTA
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                    CG
                         ASP B 297
                                           59.768
                                                    90.974
                                                             63.284
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                    OD1
                        ASP
                             В
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                                           58.741
                                                    91.689
                                                             63.212
                                                                       1.00
                                                                            38.80
    MOTA
             8174
                    OD2
                        ASP
                             В
                               297
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67.759
                                           59.939
                                                    90.109
                                                                       1.00
                                                                            38.68
             8175
    ATOM
                             B 298
                                           60.312
                    N
                         HIS
                                                    91.350
                                                                       1.00 30.55
70
    ATOM
             8176
                   CA
                        HIS B 298
                                           60.874
                                                    91.004
                                                             69.054
                                                                       1.00 30.71
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	ATOM	8177	С	HIS	В	298	60.130	89.772	69.621	1.00	29.76
	ATOM	8178	Õ	HIS			59.090	89.365	69.063	1.00	27.72
	ATOM	8179	CB	HIS			60.714	92.206	70.014		30.05
	ATOM	8180	CG	HIS			59.328	92.743	70.019		31.67
5	ATOM	8181		HIS	В	298	58.289	92.093	70.651		32.69
	ATOM	8182				298	58.778	93.807	69.387		32.54
	ATOM	8183		HIS			57.165	92.763	70.445		33.57
	MOTA	8184		HIS			57.433	93.807	69.682		32.79
10	ATOM	8185	N	TYR			60.646 60.088	89.263 88.128	70.761 71.506		28.58 27.63
10	ATOM	8186 8187	CA C	TYR TYR			59.928	88.447	72.996		27.71
	ATOM ATOM	8188	0	TYR			60.705	89.211	73.574		26.61
	ATOM	8189	СВ	TYR			61.044	86.939	71.462		27.77
	ATOM	8190	CG	TYR		299	61.450	86.482	70.086	1.00	26.03
15	ATOM	8191	CD1	TYR			60.543	85.858	69.243	1.00	25.67
	ATOM	8192	CD2	TYR	В	299	62.746	86.682	69.632	1.00	24.84
	MOTA	8193	CE1	TYR	В	299	60.930	85.444	67.989		27.49
	MOTA	8194	CE2	TYR		299	63.137	86.274	68.382		25.15
	MOTA	8195	CZ	TYR		299	62.236	85.657	67.561		25.06
20	ATOM	8196	ОН	TYR		299	62.642	85.223	66.324		24.17
	ATOM	8197	N	LEU		300	58.941	87.821 87.852	73.619 75.055		28.49 28.84
	ATOM	8198 8199	CA C	LEU LEU		300 300	58.779 59.562	86.601	75.450		29.14
	ATOM ATOM	8200	0	LEU		300	59.231	85.527	74.992		27.77
25	ATOM	8201	СВ	LEU		300	57.322	87.707	75.434		29.23
23	ATOM	8202	ČĞ	LEU		300	56.811	88.266	76.750	1.00	32.12
	ATOM	8203		LEU			55.589	87.482	77.288	1.00	32.90
	ATOM	8204	CD2	LEU	В	300	57.835	88.324	77.774		32.13
	ATOM	8205	N	CYS	В	301	60.597	86.728	76.272		29.52
30	ATOM	8206	CA	CYS		301	61.468	85.588	76.511		31.07
	ATOM	8207	C	CYS		301	61.295	85.042	78.009		33.70
	ATOM	8208	0_	CYS		301	61.457	83.843	78.255		35.22
	ATOM	8209	CB	CYS		301	62.955	85.890 85.226	75.934 74.152		31.26 27.63
25	ATOM	8210 8211	SG	CYS ASP		301	63.459 60.840	85.858	78.975		35.00
35	ATOM ATOM	8212	N CA	ASP			60.731	85.433	80.390		35.86
	ATOM	8213	C	ASP			59.799	86.343	81.231		34.62
	ATOM	8214	ŏ	ASP		302	59.860	87.545	81.093		34.73
	ATOM	8215	ČВ	ASP		302	62.139	85.511	81.022	1.00	37.25
40	MOTA	8216	CG	ASP	В	302	62.420	84.378	81.981		41.73
	MOTA	8217	OD1	ASP	В	302	61.930	84.430	83.144		44.78
	MOTA	8218		ASP		302	63.155	83.394	81.660		49.19
	ATOM	8219	N	VAL		303	58.955	85.778	82.098		33.21
4-	ATOM	8220	CA	VAL			58.075	86.546	82.968 84.410		32.77 32.40
45	ATOM ATOM	8221 8222	C O	VAL VAL		303	58.258 58.163	86.081 84.890	84.672		31.17
	ATOM	8223	СВ	VAL			56.578	86.310	82.680		33.24
	ATOM	8224		VAL			55.759				32.91
	ATOM	8225		VAL			56.218	86.597	81.232	1.00	33.73
50	ATOM	8226	N	THR	В	304	58.471	87.013	85.343		31.14
	ATOM	8227	CA	THR			58.775	86.624	86.706		31.77
	ATOM	8228	С	THR			58.112	87.603	87.658		31.80
	ATOM	8229	0	THR	В	304	58.304	88.816	87.523		32.38
	ATOM	8230	CB	THR			60.327	86.611	86.970 86.057		31.19 32.47
55	ATOM	8231	OG1	THR THR			60.992 60.633	85.722 86.006	88.314		34.29
	ATOM ATOM	8232 8233	CG2 N	TRP			57.327	87.086	88.603		31.45
	ATOM	8234	CA	TRP			56.718	87.935	89.617		31.62
	ATOM	8235	C	TRP			57.811	88.187	90.637		31.10
60	ATOM	8236	ō	TRP			58.330	87.248	91.154		31.07
•	ATOM	8237	CB	TRP			55.517	87.225	90.269	1.00	31.70
	ATOM	8238	CG	TRP	В	305	54.311	87.317	89.468	1.00	31.84
	ATOM	8239	CD1	TRP			53.852	86.405	88.560	1.00	33.39
	MOTA	8240	CD2	TRP			53.406	88.424	89.410		31.59
65	ATOM	8241		TRP			52.711	86.879	87.959		31.28
	MOTA	8242	CE2	TRP			52.419	88.116	88.470		31.64 33.06
	ATOM	8243 8244	CE3	TRP TRP			53.335 51.377	89.644 88.979	90.057 88.178		33.53
	ATOM ATOM	8244	CZ3	TRP			52.286	90.497	89.770		34.48
70	ATOM	8246		TRP			51.323	90.160	88.853		32.18
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	АТОМ	8247	N ALA	B 306	58.217	7 89.433	3 90.864	1 1 00 31 03
	ATOM	8248	CA ALA	B 306	59.201	1 89.737		
	ATOM ATOM	1777		B 306 B 306	58.518 59.051			1.00 33.56
!	5 ATOM	8251	CB ALA	B 306	59.980			
	ATOM ATOM			B 307	57.365	90.554	93.297	1.00 34.17
	ATOM			B 307 B 307	56.524 55.055			
17	ATOM		O THR	B 307	54.780	90.554		
10	ATOM ATOM			B 307 B 307	56.695 56.206			1.00 35.48
	ATOM	8258 (B 307	58.175			
	ATOM		GLN	В 308	54.120	90.631	95.034	1.00 36.50
15	ATOM ATOM		CA GLN	B 308 B 308	52.690 52.351			1.00 36.66
	ATOM	8262) GLN	B 308	51.316			
	ATOM ATOM		CB GLN	B 308 B 308	51.789		95.984	1.00 37.14
	ATOM		D GLN	B 308	52.147 51.937			1.00 37.08 1.00 40.81
20			E1 GLN	B 308	51.351	87.991		1.00 40.81 1.00 38.86
	ATOM ATOM	8267 N 8268 N	JE2 GLN	B 308 B 309	52.418 53.212		97.924	1.00 37.75
	MOTA	8269 C	A GLU	B 309	52.907	92.775 93.966	93.688 92.883	1.00 36.25 1.00 36.43
25	ATOM ATOM	8270 C 8271 C		B 309	53.954	94.349	91.879	1.00 35.70
23	ATOM		GLU B GLU		53.939 52.725	95.485 95.188	91.363 93.765	1.00 35.36
	ATOM	8273 C	G GLU	В 309	51.746	94.973	94.891	1.00 36.88 1.00 41.29
	ATOM ATOM		D GLU E1 GLU		51.386	96.277	95.577	1.00 46.84
30	MOTA	8276 O	E2 GLU	В 309	52.313 50.169	97.065 96.513	95.905 95.748	1.00 50.25 1.00 51.11
	ATOM ATOM	8277 N 8278 C			54.873	93.443	91.588	1.00 34.99
	ATOM	8278 C. 8279 C		B 310 B 310	55.907 56.220	93.777 92.582	90.620 89.759	1.00 34.77
25	ATOM	8280 O	ARG 1	B 310	56.494	91.501	90.272	1.00 34.15 1.00 34.19
35	ATOM ATOM	8281 C		B 310	57.165	94.261	91.337	1.00 34.67
	ATOM	8283 CI			58.381 59.598	94.291 94.806	90.481 91.231	1.00 34.36 1.00 37.03
	ATOM ATOM	8284 N			59.478	96.236	91.473	1.00 37.03
40	ATOM	8285 C: 8286 NI	Z ARG I H1 ARG I		60.277 60.038	96.964 98.258	92.226	1.00 40.61
	ATOM	8287 NI	H2 ARG E	3 3 1 0	61.298	96.422	92.349	1.00 42.04 1.00 41.05
	ATOM ATOM	8288 N 8289 C	ILE E		56.158	92.800	88.453	1.00 33.58
	ATOM	8290 C	ILE E	3 3 1 1	56.441 57.663	91.777 92.159	87.475 86.679	1.00 33.34 1.00 32.04
45	ATOM ATOM	8291 O 8292 CE	ILE E	3 3 1 1	57.848	93.319	86.298	1.00 31.10
	ATOM		3 ILE E 31 ILE E	3 311 3 311	55.290 53.962	91.632 91.831	86.488 87.171	1.00 33.75
	ATOM	8294 CG	32 ILE E	311	55.320	90.264	85.828	1.00 36.32 1.00 33.59
50	ATOM ATOM	8295 CI 8296 N	O1 ILE E SER E	311	52.812 58.482	91.743	86.200	1.00 38.06
	ATOM	8297 CA	SER B	312	59.650	91.162 91.365	86.401 85.576	1.00 30.98 1.00 30.92
	ATOM ATOM	8298 C 8299 O	SER B	312	59.436	90.700	84.218	1.00 30.94
	ATOM	8300 CE	SER B SER B		59.183 60.824	89.489 90.703	84.163 86.242	1.00 31.01 1.00 30.36
55	ATOM	8301 OG	SER B	312	61.950	91.004	85.505	1.00 30.36
	ATOM ATOM	8302 N 8303 CA	LEU B		59.540 59.361	91.468 90.929	83.139	1.00 31.72
	ATOM	8304 C	LEU B	313	60.658	91.067	81.780 81.018	1.00 31.65 1.00 31.48
60	ATOM ATOM	8305 O 8306 CB	LEU B		61.245	92.154	80.953	1.00 31.36
00	ATOM	8307 CG		313	58.273 56.897	91.687 91.696	81.038	1.00 32.02
	ATOM	8308 CD	1 LEU B	313	56.013	92.618	81.697 80.928	1.00 33.58 1.00 33.88
	ATOM ATOM	8309 CD 8310 N	2 LEU B GLN B		56.267	90.298	81.757	1.00 35.31
65	ATOM	8311 CA			61.129 62.364	89.979 90.044	80.454 79.708	1.00 30.90 1.00 31.97
	ATOM	8312 C	GLN B	314	62.066	89.884	78.215	1.00 31.97
	ATOM ATOM	8313 O 8314 CB	GLN B GLN B		61.493 63.364	88.884 89.018	77.814	1.00 32.91
70	ATOM	8315 CG	GLN B	314	64.795	89.386	80.210 79.861	1.00 31.34 1.00 35.07
70	ATOM	8316 CD	GLN B	314	65.863	88.543	80.626	1.00 35.88

	MOTA	8317		GLN E		67.037	88.877	80.607	1.00 37.83
	ATOM	8318	NE2			65.443	87.481	81.274	1.00 36.84 1.00 30.58
	ATOM ATOM	8319 8320	N CA	TRP E		62.408 62.148	90.904 90.949	77.437 76.010	1.00 30.58 1.00 30.91
5	ATOM	8321	C	TRP E		63.425	90.754	75.234	1.00 29.95
_	ATOM	8322	ō	TRP E		64.484	91.034	75.744	1.00 31.13
	ATOM	8323	CB	TRP F	315	61.521	92.302	75.597	1.00 30.37
	MOTA	8324	CG	TRP E		60.236	92.639	76.303	1.00 31.01
	MOTA	8325	CD1			60.102	93.311	77.494	1.00 32.19
10	ATOM	8326	CD2			58.904	92.327	75.881	1.00 30.33
	ATOM ATOM	8327 8328	NE1 CE2			58.777 58.025	93.424 92.848	77.820 76.839	1.00 30.77 1.00 29.77
	ATOM	8329	CE3			58.365	91.655	74.776	1.00 29.77
	ATOM	8330	CZ2			56.646	92.716	76.741	1.00 32.04
15	ATOM	8331	CZ3			57.014	91.527	74.681	1.00 31.97
	ATOM	8332	CH2			56.162	92.050	75.655	1.00 31.73
	ATOM	8333	N	LEU E	316	63.319	90.296	73.996	1.00 29.83
	ATOM	8334	CA	LEU E		64.495	90.080	73.131	1.00 31.28
20	ATOM	8335	C	LEU E		64.189	90.512	71.687	1.00 31.65
20	ATOM	8336 8337	O	LEU E		63.095 64.932	90.273 88.610	71.174 73.164	1.00 31.45 1.00 30.42
	MOTA ATOM	8338	CB CG	LEU B		66.108	88.062	72.350	1.00 30.42 1.00 33.06
	ATOM	8339	CD1			67.422	88.670	72.724	1.00 33.00
	ATOM	8340	CD2			66.158	86.509	72.506	1.00 34.10
25	ATOM	8341	N	ARG B	317	65.147	91.171	71.047	1.00 33.19
	ATOM	8342	CA	ARG B		64.979	91.553	69.659	1.00 34.37
	ATOM	8343	C	ARG B		65.123	90.335	68.784	1.00 33.87
	ATOM	8344	0	ARG B		65.815	89.380	69.140	1.00 34.03
30	ATOM ATOM	8345 8346	CB CG	ARG B		65.996 65.670	92.625 94.068	69.277 69.853	1.00 36.07 1.00 37.65
30	ATOM	8347	CD	ARG B		66.288	95.194	68.990	1.00 37.03
	ATOM	8348	NE	ARG B		66.022	96.529	69.532	1.00 40.43
	ATOM	8349	CZ	ARG B		66.934	97.509	69.653	1.00 40.38
	ATOM	8350	NH1	ARG B	317	68.199	97.337	69.241	1.00 37.57
35	MOTA	8351	NH2		317	66.568	98.677	70.180	1.00 37.66
	ATOM	8352	N	ARG B	318	64.436	90.339	67.652	1.00 33.75
	ATOM	8353	CA	ARG B	318	64.582	89.259	66.696	1.00 33.76
	MOTA MOTA	8354 8355	C O	ARG B	318 318	66.031 66.533	89.091 87.974	66.348 66.209	1.00 34.27 1.00 35.49
40	ATOM	8356	СВ	ARG B		63.749	89.501	65.431	1.00 33.49
10	ATOM	8357	CG	ARG B	318	63.566	88.230	64.624	1.00 32.42
	ATOM	8358	CD	ARG B	318	62.759	88.436	63.348	1.00 32.20
	ATOM	8359	NE	ARG B	318	62.754	87.234	62.545	1.00 31.52
	MOTA	8360	CZ	ARG B	318	61.754	86.850	61.757	1.00 26.85
45	ATOM	8361	NH1	ARG B	318	60.670	87.581	61.616	1.00 25.05
	ATOM	8362	NH2		318	61.859	85.718	61.113	1.00 27.58
	ATOM ATOM	8363 8364	N CA	ILE B		66.721 68.178	90.187 90.117	66.138 66.032	1.00 35.43 1.00 36.02
	ATOM	8365	C	ILE B	319	68.609	89.953	67.496	1.00 35.99
50	ATOM	8366	ō	ILE B	319	68.636	90.912	68.248	1.00 36.06
	MOTA	8367	CB	ILE B	319	68.699	91.387	65.382	1.00 36.52
	MOTA	8368	CG1	ILE B		68.314	91.373	63.903	1.00 39.38
	ATOM	8369	CG2	ILE B		70.197	91.477	65.464	1.00 38.69
==	MOTA	8370	CD1	ILE B		68.390	92.774	63.236	1.00 42.38
55	ATOM ATOM	8371 8372	N CA	GLN B	320 320	68.944 69.067	88.730 88.366	67.889 69.300	1.00 35.86 1.00 36.22
	ATOM	8373	C	GLN B		70.372	88.820	69.962	1.00 36.22
	ATOM	8374	ŏ	GLN B		71.063	88.031	70.624	1.00 36.55
	ATOM	8375	ČВ	GLN B		68.848	86.863	69.443	1.00 35.91
60	ATOM	8376	CG	GLN B	320	67.536	86.390	68.779	1.00 36.08
	ATOM	8377	CD	GLN B		67.310	84.878	68.855	1.00 37.12
	ATOM	8378	OE1	GLN B		67.791	84.200	69.778	1.00 33.28
	ATOM	8379	NE2	GLN B		66.569	84.344	67.870	1.00 37.03
65	MOTA	8380	N	ASN B		70.603	90.124	69.816	1.00 36.83
65	ATOM ATOM	8381 8382	CA C	ASN B		71.791 71.561	90.866 91.766	70.229 71.422	1.00 37.99 1.00 36.96
	ATOM	8383	Ö	ASN B		72.496	92.360	71.422	1.00 36.30
	ATOM	8384	СВ	ASN B		72.175	91.860	69.080	1.00 37.62
	MOTA	8385	CG	ASN B		73.398	91.459	68.385	1.00 41.47
70	ATOM	8386	OD1	ASN B		74.024	90.479	68.794	1.00 51.40

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ATOM
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       ATOM
               8388
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                            TYR
                                B 322
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       ATOM
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                      CA
                            TYR
                                B 322
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       ATOM
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                            TYR B 322
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       ATOM
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       MOTA
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                      CG
                            TYR B
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       ATOM
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                                              70.357
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                           TYR B
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72.761
                                                        96.402
                                                                           1.00 35.79
               8395
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                                                                           1.00
                                                                                  35.35
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                           TYR B 322
                                              70.102
                                                        97.614
                                                                  73.393
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                                              67.799
68.822
       ATOM
               8397
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                           TYR B 322
                                                        97.071
                                                                  73.418
                                                                           1.00 37.85
      ATOM
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                      CZ
                           TYR B
                                  322
                                                                 73.726
74.380
                                                        97.938
                                                                           1.00 37.94
      ATOM
               8399
                      OH
                           TYR B 322
                                              68.509
                                                       99.110
                                                                           1.00 39.12
      ATOM
               8400
                                              68.690
67.581
67.423
                      N
                           SER B 323
                                                       92.688
                                                                 74.672
                                                                           1.00 34.97
 15
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               8401
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                           SER B 323
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                                                                 75.511
                                                                           1.00 34.88
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               8402
                           SER B 323
                                                                 76.600
77.047
                      С
                                                       93.386
                                                                           1.00 34.54
      ATOM
               8403
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                           SER B 323
                                              68.352
                                                       94.026
                                                                           1.00 33.93
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                           SER B 323
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                                                       90.979
                                                                 76.161
                                                                           1.00 34.56
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               8405
                           SER B 323
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                                                       90.954
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                                                                           1.00 36.68
 20
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65.787
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77.996
                      Ν
                           VAL B 324
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                           VAL B 324
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1.00 35.00
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1.00 35.00
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                                                                 76.361
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                                                       96.292
                                             65.165
64.326
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               8413
                      N
                           MET
                               В
                                  325
                                                       93.885
                                                                           1.00 35.13
                                                                 80.226
      ATOM
               8414
                           MET B 325
                      CA
                                                                 81.296
81.759
                                                       93.430
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              8415
                           MET B
                                  325
                                             63.537
                                                       94.679
                      C
                                                                           1.00 36.30
 30
      ATOM
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                           MET B 325
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65.227
64.619
                                                       95.719
92.906
                      0
                                                                 82.062
                                                                           1.00 35.13
              8417
      ATOM
                                                                 82.409
83.381
84.519
                      CB
                           MET
                               В
                                  325
                                                                           1.00 37.09
      ATOM
              8418
                               В
                                  325
                      CG
                           MET
                                                       91.939
                                                                           1.00 40.89
      ATOM
              8419
                      SD
                           MET B
                                  325
                                             65.964
                                                       91.400
                                                                           1.00
                                                                                 44.02
      ATOM
              8420
                           MET B 325
                      CE
                                             65.131
                                                       91.287
                                                                 85.946
                                                                          1.00
                                                                                 41.92
                                             62.206
61.339
60.755
 35
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                               В
                                  326
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                                                                 81.759
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                                                       95.665
95.336
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83.531
                     CA
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                                                                          1.00
                                                                                36.76
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                     C
                           ASP
                               B 326
                                                                          1.00
                                                                                 36.82
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                           ASP B 326
                                             60.292
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                                                                                 36.86
                                                                          1.00
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59.940
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              8425
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97.198
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                          ASP
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                                                                          1.00
                                                                                 37.27
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                     CG
                          ASP
                               В
                                  326
                                                                 80.757
81.246
                                                                          1.00
                                                                                40.61
     ATOM
              8427
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                          ASP
                                  326
                                             60.662
                                                       98.086
                               В
                                                                          1.00
                                                                                 43.19
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60.748
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                                                                          1.00
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                     N
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                                                                                36.94
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                     CA
                          ILE
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                                                                                37.80
45
     ATOM
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                     С
                           ILE
                               В
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     ATOM
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                                                                          1.00
                                                                                38.44
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62.305
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                          ILE
                               В
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                                                                86.767
                                                                          1.00
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                          ILE
                               В
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                                                                86.660
                                                                          1.00
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                                             60.678
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                          ILE
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                                                                                38.82
50
     ATOM
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                               B 327
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                                                                86.910
                                                                          1.00 41.48
                                            57.843
56.525
     ATOM
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                          CYS
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                                 328
                                                      96.182
96.784
                                                                86.157
                                                                          1.00 39.11
     MOTA
              8438
                                 328
                     CA
                          CYS
                               В
                                                                86.136
87.478
                                                                          1.00 40.17
     ATOM
              8439
                     С
                          CYS B 328
                                             55.810
                                                      96.662
                                                                          1.00 40.31
     ATOM
              8440
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                          CYS B 328
                                             55.657
                                                      95.574
                                                                88.012
                                                                          1.00 39.11
55
                                                      96.150
96.102
97.803
     ATOM
                                            55.695
56.529
              8441
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                          CYS
                               В
                                 328
                                                                85.032
                                                                          1.00 39.94
     ATOM
              8442
                          CYS B
                                                                83.429
87.971
                     SG
                                 328
                                                                          1.00 43.57
     ATOM
              8443
                     N
                          ASP B
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                     CA
                          ASP B 329
                                            54.739
                                                      97.898
                                                                89.300
                                                                          1.00 42.47
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             8445
                          ASP B
                                 329
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                                            53.266
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                                                                          1.00 43.58
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                     0
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                                                                          1.00 43.63
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                          ASP B 329
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                    CG
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                                                                          1.00 43.42
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                     OD1 ASP B 329
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97.463
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                         ASP
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                                                                          1.00 45.24
65
     MOTA
             8451
                    N
                                 330
                                            52.509
                          TYR B
                                                                90.068
                                                                          1.00 45.51
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                    CA
                          TYR B 330
                                            51.080
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     MOTA
             8453
                    C
                          TYR B 330
                                            50.792
                                                      99.073
                                                                90.787
                                                                          1.00 49.73
    ATOM
             8454
                                            51.414
50.361
                    0
                          TYR
                              В
                                 330
                                                      99.436
                                                                91.778
                                                                          1.00 48.59
    ATOM
             8455
                    CB
                          TYR B 330
                                                      96.626
                                                                90.924
                                                                          1.00 48.00
70
    ATOM
             8456
                    CG
                          TYR B 330
                                            48.883
                                                      96.872
                                                                90.940
                                                                          1.00 49.60
```

	ATOM ATOM	8457 8458	CD1 CD2			330 330	48.186 48.182		89.750 92.132	1.00 52.40 1.00 49.68
	ATOM	8459	CE1				46.829		89.752	1.00 51.02
	ATOM	8460	CE2			330	46.831	97.198	92.141	1.00 51.01
5	ATOM	8461	CZ	TYR	В	330	46.170	97.381	90.947	1.00 50.55
	ATOM	8462	OH			330	44.838		90.945	1.00 52.45
	MOTA	8463	N			331	49.863		90.199	1.00 52.21
	ATOM	8464	CA			331		101.142	90.731	1.00 54.21
	ATOM	8465	C			331		101.135	91.443	1.00 55.17
10	ATOM	8466	0			331		101.105	90.809	1.00 54.64
	MOTA	8467	СВ			331		102.188	89.616	1.00 54.82
	MOTA	8468	CG	ASP		331		103.623 103.797	90.159 91.402	1.00 56.20 1.00 57.58
	MOTA	8469			-	-		103.797		1.00 57.38
16	MOTA	8470	OD2	ASP GLU		331		104.630	89.417 92.764	1.00 55.34
15	ATOM ATOM	8471 8472	N CA	GLU				101.164	93.634	1.00 57.04
	ATOM	8473	C	GLU		332		102.249	93.098	1.00 58.60
	ATOM	8474	Ö			332		101.938	93.040	1.00 58.62
	ATOM	8475	ČВ	GLU		332		101.647	95.064	1.00 59.12
20	ATOM	8476	ĊĞ			332		103.075	95.550	1.00 61.50
	ATOM	8477	CD	GLU		332		103.648	96.544	1.00 63.70
	ATOM	8478	OE1	GLU	В	332	48.425	103.040	97.621	1.00 63.97
	ATOM	8479	OE2	GLU	В	332	48.785	104.733	96.254	1.00 64.40
	MOTA	8480	N	SER				103.424	92.677	1.00 59.26
25	ATOM	8481	CA	SER		333		104.481	92.182	1.00 59.33
	MOTA	8482	С	SER		333		104.118	90.856	1.00 59.48
	ATOM	8483	0	SER		333		103.946	90.745	1.00 60.00
	ATOM	8484	CB	SER		333		105.789	91.992	1.00 59.31
20	MOTA	8485	OG	SER		333		106.327	93.225	1.00 59.60
30	ATOM	8486	N	SER				104.027 103.794	89.841 88.464	1.00 59.75 1.00 59.29
	ATOM ATOM	8487 8488	CA C	SER SER		334		103.794	88.202	1.00 58.62
	ATOM	8489	Ö	SER		334		102.424	87.321	1.00 58.02
	ATOM	8490	СВ	SER		334		103.984	87.535	1.00 59.95
35	ATOM	8491	OG	SER		334		102.813	86.757	1.00 60.68
-	ATOM	8492	N	GLY		335		101.424	88.966	1.00 57.60
	ATOM	8493	CA	GLY		335		100.056	88.676	1.00 56.75
	ATOM	8494	C	GLY		335	45.530	99.590	87.413	1.00 55.98
	MOTA	8495	0	GLY	В	335	45.144	98.612	86.786	1.00 55.77
40	ATOM	8496	N	ARG				100.312	87.001	1.00 55.26
	ATOM	8497	CA	ARG			47.340		85.849	1.00 55.10
	MOTA	8498	C	ARG			48.786		86.214	1.00 53.48
	ATOM	8499	0	ARG		336	49.166		87.390	1.00 53.40
45	ATOM	8500	CB	ARG ARG		336		100.861	84.686 83.991	1.00 55.82 1.00 58.15
45	ATOM ATOM	8501 8502	CG CD	ARG		336 336		100.694 101.645	82.855	1.00 58.15
	ATOM	8503	NE	ARG				101.486	82.401	1.00 65.16
	ATOM	8504	CZ	ARG				100.932	81.248	1.00 67.78
	ATOM	8505		ARG				100.482	80.388	1.00 67.72
50	ATOM	8506		ARG			42.540		80.952	1.00 67.74
	ATOM	8507	N	TRP			49.579	99.242	85.209	1.00 51.65
	ATOM	8508	CA	TRP			50.931	98.806	85.452	1.00 50.02
	ATOM	8509	С	TRP			51.925	99.718	84.765	1.00 50.23
	ATOM	8510	0	TRP			51.857	99.882	83.556	1.00 50.77
55	MOTA	8511	СВ	TRP			51.077	97.379	84.940	1.00 49.16
	ATOM	8512	CG	TRP			50.349	96.355	85.753	1.00 44.51
	ATOM	8513		TRP			49.075	95.930	85.582	1.00 39.99
	ATOM ATOM	8514	CD2	TRP TRP			50.869 48.767	95.618 94.970	86.868 86.514	1.00 39.72 1.00 38.99
60		8515 8516		TRP			49.860	94.757	87.310	1.00 38.99
60	ATOM ATOM	8517	CE3				52.090	95.593	87.521	1.00 37.17
	ATOM	8518		TRP			50.033	93.896	88.373	1.00 37.17
	ATOM	8519	CZ3				52.270	94.735	88.557	1.00 37.64
	ATOM	8520		TRP			51.247	93.898	88.983	1.00 37.04
65	ATOM	8521	N	ASN			52.842		85.541	1.00 49.98
	ATOM	8522	CA	ASN			53.878		85.024	1.00 49.89
	ATOM	8523	C	ASN			55.257		85.007	1.00 49.40
	ATOM	8524	0	ASN			55.649	99.926	85.961	1.00 49.36
	ATOM	8525	CB	ASN			53.944	102.484	85.865	1.00 49.80
70	ATOM	8526	CG	ASN			52.696	103.329	85.718	1.00 51.11

	ATOM ATOM	8528	ND2 A	ASN	B 338 B 338	52.030	2 103.707 0 103.611	86.847	1.00	50.56 47.68
	ATOM ATOM	8529 8530			B 339 B 339	55.961	l 100.768 9 100.212	83.905	1.00	49.38
5	MOTA	8531			B 339	58.205	100.212	83.685 83.455		49.73
	ATOM	8532			B 339	58.305	101.916	82.340	1.00	50.56
	ATOM ATOM	8533 8534		-	B 339 B 339	57.337 56.155			1.00	49.43
	ATOM	8535			B 340		37.857 3 101.876		1.00	47.42 50.25
10		8536	CA I	EU I	B 340	59.744	103.020	84.431	1.00	50.23
	MOTA ATOM	8537 8538			B 340 B 340	60.955	102.752	83.556	1.00	50.03
	ATOM	8539			340	60.216	101.891 103.430	83.832 85.825	1.00	49.59 51.05
1.5	ATOM	8540	CG L	EU I	3 3 4 0	59.748	104.746	86.446		52.01
15	ATOM ATOM	8541 8542	CD1 L			58.249	104.940	86.344	1.00	54.40
	ATOM	85 4 2	CD2 L		3 340		104.750 103.541	87.902 82.506	1.00	53.37 50.16
	MOTA	8544			3 3 4 1		103.400	81.585	1.00	50.16
20	ATOM ATOM	8545			3 3 4 1	63.565	103.419	82.240	1.00	49.64
20	ATOM	8546 8547	O V	AL E	3 341 3 341	64.471	102.692 104.493	81.817	1.00	49.50
	ATOM	8548	CG1 V	AL E	3 3 4 1	63.501	104.493	80.532 79.847		50.32 50.95
	ATOM ATOM	8549	CG2 V	AL E	3 3 4 1	61.020	104.205	79.513	1.00	51.51
25	ATOM	8550 8551			3 342 3 342	63.746	104.222 104.348	83.275		48.96
	ATOM	8552	C A	LA E	342	65.420	104.348	83.826 84.638		48.51 47.95
	ATOM	8553	O A	LA E	342	66.568	102.921	85.011	1.00	48.49
	ATOM ATOM	8554 8555		LA E		65.232	105.631 102.278	84.654	1.00	48.86
30	ATOM	8556		RG B		64.668	102.278	84.875 85.687		47.01 46.47
	ATOM	8557		RG B	343	64.755	99.795	84.816		45.21
	ATOM ATOM	8558 8559		RG B		64.712	98.683	85.302		44.07
	ATOM			RG B		63.260	101.071 99.809	86.782 87.425		46.53 47.76
35	ATOM		CD A	RG B	343	61.939	99.939	88.173		49.49
	ATOM ATOM			RG B	343 343	62.057 61.039	100.749	89.374		51.13
	ATOM		NH1 AI			59.819	101.378 101.320	89.974 89.455		53.68 54.07
40	ATOM				343	61.241	102.078	91.093		52.56
40	ATOM ATOM		N GI CA GI	N B	344 344	64.920 65.117	99.987	83.517		44.33
	ATOM				344	66.514	98.889 98.317	82.586 82.736	1.00	43.95 43.83
	ATOM				344	67.463	99.061	82.880	1.00	43.78
45	ATOM ATOM				344 344	64.986 63.550	99.396	81.122		43.32
	ATOM				344		99.535 100.271	80.623 79.278	$1.00 \\ 1.00$	
	ATOM	8573	OE1 GI	N B	344	64.364	100.388	78.534	1.00	
	MOTA MOTA		NE2 GI N HI		344 345		100.727	78.979	1.00	
50	ATOM				345	66.664 68.009	97.003 96.443	82.683 82.590	$1.00 \\ 1.00$	44.19
	ATOM		C HI	S B	345	68.256	95.843	81.221	1.00	43.03
	ATOM ATOM			S B S B	345 345	67.430	95.099	80.700	1.00	43.19
	ATOM	8580 (345	68.320 68.718	95.537 96.323	83.760 84.975	1.00	
55	MOTA		ND1 HI	SB	345	67.873	96.529	86.048	1.00	
	ATOM ATOM		CD2 HI		345	69.851	97.019	85.246	1.00	51.01
	ATOM		CE1 HI NE2 HI		345 345	68.486 69.683	97.279 97.597	86.948 86.480	1.00	
	MOTA	8585 n	N IL		346	69.396	96.226	80.648	1.00	41.59
60	ATOM ATOM				346	69.757	95.956	79.267	1.00	41.02
	ATOM				346 346	70.982 71.973	95.099 95.327	79.127	1.00	
	ATOM	8589 C	CB IL	Е В	346	70.050	97.301	79.790 78.577	1.00	
65	ATOM			ЕВ		68.815	98.189	78.604	1.00	42.09
U.J	ATOM ATOM			E B E B	346 346	70.507 69.057	97.096 99.578	77.141	1.00	
	MOTA	8593 N		ЈВ	347	70.910	94.080	78.042 78.292	1.00 4	
	ATOM		CA GL	ЈВ	347	72.074	93.254	78.001	1.00 4	
70	ATOM ATOM	8595 C		J B J B	347 347	72.243	93.244	76.498	1.00 4	
		3370 0	اللق	ם כ	J4/	71.252	93.214	75.761	1.00 4	11.58

	ATOM ATOM	8597 8598	CB CG		3 47 3 347	71.909 71.613	91.820 91.647	78.463 79.925		41.54 42.14
	ATOM	8599	CD		3 347	71.340	90.199	80.249		42.92
	ATOM	8600	OE1		3 347	71.894	89.339	79.524		40.30
5	ATOM	8601	OE2		3 3 4 7	70.611	89.932	81.245		43.22
•	ATOM	8602	N		3 3 4 8	73.497	93.293	76.063		42.77
	ATOM	8603	CA		3 3 4 8	73.847	93.338	74.670	1.00	43.61
	MOTA	8604	С	MET I	3 3 4 8	75.009	92.412	74.520	1.00	43.46
	ATOM	8605	0		3 3 4 8	75.694	92.113	75.477	1.00	41.97
10	MOTA	8606	СВ		3 3 4 8	74.345	94.728	74.243		44.65
	ATOM	8607	CG		3 3 4 8	73.612	95.910	74.808		47.60
	ATOM	8608	SD		3 3 4 8	73.971	97.448	73.889		54.54
	ATOM	8609	CE	MET I		73.036	98.636	74.807		55.02
1.5	ATOM	8610	N		3 3 4 9	75.240	91.944	73.312		44.14
15	ATOM	8611 8612	CA C		3 3 4 9 3 3 4 9	76.439 77.087	91.164 91.677	73.078 71.836		45.08 45.42
	ATOM ATOM	8613	Ö		349	76.417	92.017	70.862		45.19
	ATOM	8614	СВ		3 3 4 9	76.131	89.677	72.911		45.44
	ATOM	8615	OG		349	77.328	88.900	72.852		45.77
20	ATOM	8616	N		350	78.403	91.742	71.876		46.25
	ATOM	8617	CA	THR E		79.156	92.062	70.682		46.88
	ATOM	8618	С	THR E	3 3 5 0	79.737	90.764	70.158	1.00	46.10
	MOTA	8619	0	THR E	350	79.806	90.559	68.952		47.60
	ATOM	8620	CB	THR E		80.264	93.119	70.981		47.27
25	MOTA	8621	OG1			79.877	94.396	70.448		48.80
	ATOM	8622	CG2	THR E		81.510	92.828	70.216		48.44
	ATOM	8623	N	THR E		80.103	89.867	71.065		44.83
	ATOM	8624	CA	THR E		80.770	88.623	70.704		44.31
30	ATOM	8625 8626	C O	THR E		79.832 80.258	87.607 86.796	69.986 69.166		42.17 41.47
30	ATOM ATOM	8627	СВ	THR E		81.387	88.060	72.004		45.00
	ATOM	8628	OG1	THR E		82.318	89.023	72.529		48.79
	ATOM	8629	CG2	THR E		82.282	86.861	71.767		46.07
	ATOM	8630	N	GLY E		78.542	87.671	70.267		39.36
35	ATOM	8631	CA	GLY E		77.638	86.685	69.715		37.02
	ATOM	8632	C	GLY E		76.230	86.990	70.099	1.00	34.71
	MOTA	8633	0	GLY E	352	75.762	88.057	69.773		33.50
	MOTA	8634	N	TRP E		75.573	86.073	70.815		32.66
	ATOM	8635	CA	TRP E		74.176	86.260	71.159		31.41
40	ATOM	8636	C	TRP E		73.994	86.437	72.646		31.25
	ATOM	8637	0	TRP E		74.958	86.404	73.415		31.98
	ATOM ATOM	8638 8639	CB	TRP E		73.325 73.819	85.102 83.802	70.607 71.120		31.08 28.71
	ATOM	8640	CG CD1	TRP E		73.403	83.170	72.216		27.12
45	ATOM	8641	CD2	TRP E		74.843	83.009	70.563		25.31
10	ATOM	8642	NE1	TRP E		74.118	82.023	72.394		26.82
	ATOM	8643	CE2	TRP E		74.998	81.898	71.373	1.00	25.30
	ATOM	8644	CE3	TRP E	353	75.624	83.105	69.428		22.97
	ATOM	8645	CZ2	TRP E	353	75.929	80.904	71.113		24.59
50	ATOM	8646	CZ3	TRP E		76.557	82.129	69.184		23.91
	ATOM	8647	CH2	TRP E		76.694	81.039	70.020		20.31
	MOTA	8648	N	VAL E		72.771	86.682	73.074		31.63
	MOTA	8649	CA	VAL E		72.506	86.887	74.500		32.39
55	MOTA	8650	C	VAL E		72.115	85.591	75.189		32.75
55	ATOM	8651 8652	O CB	VAL E		71.120 71.338	85.006 87.819	74.814 74.701		32.29 32.04
	ATOM ATOM	8653		VAL E		71.338	88.057	76.202		32.87
	ATOM	8654		VAL E		71.593	89.112	73.948		33.99
	ATOM	8655	N	GLY E		72.887	85.167	76.189		31.57
60	ATOM	8656	CA	GLY E		72.635	83.934	76.909		32.00
	ATOM	8657	C	GLY E		73.115	82.677	76.207		32.28
	ATOM	8658	ŏ	GLY E		73.858	82.730	75.246		32.47
	ATOM	8659	N	ARG E		72.718	81.525	76.715		33.25
	ATOM	8660	CA	ARG E	356	73.065	80.266	76.074		34.63
65	ATOM	8661	С	ARG E		72.014	79.978	75.026		34.42
	MOTA	8662	0	ARG E	356	72.204	80.281	73.864	1.00	35.19
	MOTA	8663	CB	ARG E		73.173	79.159	77.121		34.64
	MOTA	8664	CG	ARG E		74.475	79.292	77.933		35.41
	MOTA	8665	CD	ARG E		74.571	78.329	79.080		35.52
70	ATOM	8666	NE	ARG B	356	75.793	78.531	79.846	1.00	38.21

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-	ATOM	8740	CE2		_	63.385	91.681	90.314	1.00 31.45
5	ATOM	8741 8742	CZ	PHE B		63.179 65.498	91.048 88.889	89.107 95.180	1.00 28.43 1.00 30.02
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	ATOM	8745	ŏ	THR B		63.203	89.406	96.319	1.00 32.79
10	ATOM	8746	ČВ	THR B		66.180	90.081	97.159	1.00 31.27
	ATOM	8747	OG1			65.607	91.202	96.482	1.00 28.45
	ATOM	8748	CG2	THR B		67.593	90.095	96.767	1.00 33.17
	ATOM	8749	N	LEU B		63.778	88.542	98.288	1.00 33.65
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15	ATOM	8751	C	LEU B		61.714	89.899 89.936	98.692	1.00 34.24
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20	ATOM	8756		LEU B	366	61.191	87.466	102.408	1.00 41.28
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25	ATOM	8761	CB	ASP B		62.381	93.386	99.544	1.00 34.77
	ATOM ATOM	8762 8763	CG OD1	ASP B	367	63.844 64.185	93.626 93.593	99.136 97.906	1.00 38.12 1.00 37.36
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30	ATOM	8766	CA	GLY B	368	61.976	92.413	94.912	1.00 33.37
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	ATOM	8769	N	ASN B	369	63.658	94.091	95.415	1.00 32.97
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35	ATOM	8771	C	ASN B	369	65.768	94.991	94.482	1.00 30.68
	ATOM ATOM	8772 8773	O CB	ASN B	369 369	66.471 64.692	95.905 96.083	94.109 96.380	1.00 29.88 1.00 33.68
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40	MOTA	8776		ASN B	369	63.460	97.500	97.902	1.00 44.89
	MOTA	8777	N	SER B	370	66.132	93.730	94.381	1.00 29.62
	MOTA	8778	CA	SER B		67.354	93.402	93.711	1.00 28.42
	MOTA	8779	C	SER B		67.210	91.984	93.213	1.00 27.80
45	ATOM	8780	0	SER B		66.286	91.264	93.617	1.00 28.01
45	ATOM ATOM	8781 8782	CB	SER B	370	68.521	93.509	94.679 95.682	1.00 27.82 1.00 28.71
	ATOM	8783	OG N	PHE B		68.386 68.140	92.513 91.571	92.370	1.00 26.71
	ATOM	8784	CA	PHE B		68.122	90.218	91.872	1.00 26.51
	ATOM	8785	C	PHE B		69.476	89.724	91.429	1.00 25.96
50	ATOM	8786	Õ		371	70.433	90.494	91.261	1.00 26.04
	ATOM	8787	СВ		371	67.163	90.106	90.712	1.00 25.97
	ATOM	8788	CG	PHE B		67.525	90.965	89.516	1.00 26.30
	MOTA	8789	CD1		371	67.081	92.277	89.425	1.00 26.19
	ATOM	8790		PHE B		68.305	90.470	88.493	1.00 26.20
55	ATOM	8791	CE1		371	67.366	93.056	88.336	1.00 28.41
	ATOM ATOM	8792 8793	CE2 CZ	PHE B	371 371	68.589 68.126	91.241 92.543	87.380 87.299	1.00 25.01 1.00 26.85
	ATOM	8794	N	TYR B		69.560	88.422	91.244	1.00 25.84
	ATOM	8795	CA	TYR B		70.807	87.819	90.776	1.00 26.43
60	ATOM	8796	C	TYR B		70.592	87.159	89.421	1.00 27.24
	ATOM	8797	0	TYR B		69.539	86.583	89.167	1.00 27.59
	ATOM	8798	CB	TYR B	372	71.299	86.800	91.791	1.00 26.09
	ATOM	8799	CG	TYR B		71.576	87.370	93.136	1.00 25.58
	ATOM	8800	CD1	TYR B	372	70.561	87.609	94.014	1.00 25.70
65	ATOM	8801	CD2	TYR B	372	72.871	87.683	93.539	1.00 27.45
	ATOM	8802			372	70.812	88.117	95.313	1.00 25.19
	ATOM ATOM	8803 8804	CE2 CZ	TYR B	372 372	73.130 72.080	88.184 88.414	94.830 95.693	1.00 27.08 1.00 28.33
	ATOM	8805	OH	TYR B		72.080	88.915	96.950	1.00 28.33
70	ATOM	8806	N	LYS B		71.611	87.194	88.572	1.00 27.72
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	ATOM ATOM ATOM		3 C		B 373 B 373 B 373	71.473 72.840 73.867	86.29	86.698	3 1.0	
5	ATOM ATOM	8810 8811 8812 8813	CG CD CE	LYS LYS LYS	B 373 B 373	70.877 70.197 69.538 68.950	7 87.824 7 87.434 8 88.673	86.341 85.077 884.427	1.00	
10	ATOM	8814 8815 8816 8817	N CA C	ILE ILE ILE	B 373 B 374 B 374 B 374	69.803 72.839 74.059 74.259	87.650 85.245 84.780 85.606	82.077 85.895 85.249	1.00 1.00 1.00	31.51 27.56 27.63 27.86
15	ATOM ATOM ATOM ATOM ATOM	8818 8819 8820 8821 8822	СВ	ILE ILE	B 374 B 374 B 374 B 374 B 374	73.350 73.963 73.842 75.160	83.320 82.470 82.917	84.883 86.148 84.002	1.00 1.00 1.00	26.36 27.04 27.49 28.04
20	ATOM ATOM ATOM ATOM	8823 8824 8825 8826	N CA C	ILE ILE ILE	B 375	73.590 75.478 75.851 77.305 78.086	86.053 86.968 86.726	83.817 82.760 82.465	1.00 1.00 1.00	27.19 29.57 30.61 30.53 29.58
25	ATOM ATOM ATOM ATOM	8827 8828 8829 8830	CB CG1 CG2 CD1	ILE ILE ILE	B 375 B 375 B 375 B 375	75.602 74.191 76.591 73.602	88.438		1.00 1.00 1.00	31.78 33.37 31.79 34.82
25	ATOM ATOM ATOM ATOM	8831 8832 8833 8834	N CA C	SER SER SER	B 376 B 376 B 376	77.646 78.992 79.913 79.617	86.930 86.734 87.823 89.003	81.202 80.730 81.270 81.142	1.00 1.00 1.00	30.08 30.69 30.51 29.37
30	ATOM ATOM ATOM ATOM ATOM	8835 8836 8837 8838 8839	CB OG N CA C	ASN ASN	B 376 B 376 B 377 B 377 B 377	78.973 80.189 81.026 81.927	86.729 86.251 87.440 88.467	79.200 78.714 81.884 82.464	1.00 1.00 1.00	30.58 32.76 31.48 32.07
35	ATOM ATOM ATOM ATOM	8840 8841 8842 8843	O CB CG OD1		B 377 B 377 B 377	82.887 82.818 82.631 83.804 84.375	89.002 88.558 87.984 87.047 86.530	81.385 80.262 83.751 83.496	1.00 1.00 1.00	32.94 32.30 30.65 29.57
40	ATOM ATOM ATOM	8844 8845 8846 8847	ND2 N CA C	ASN : GLU : GLU :	B 377 B 378 B 378 B 378	84.196 83.724 84.634 85.590	86.849 89.977 90.586 89.559	84.451 82.243 81.718 80.743 80.127	1.00 1.00 1.00	29.05 21.88 34.32 35.84 35.27
45	ATOM ATOM ATOM ATOM ATOM	8848 8849 8850 8851 8852	O CB CG CD OE1	GLU I GLU I GLU I GLU I	B 378 B 378 B 378	86.042 85.353 84.435 84.928 86.144	89.730 91.833 93.079 94.334 94.551	79.014 81.338 81.291 82.059 82.247	1.00 1.00 1.00	34.81 36.36 40.98 45.85 48.23
50	ATOM ATOM ATOM	8853 8854 8855 8856	OE2 N CA C	GLU E GLU E GLU E	3 378 3 379 3 379 3 379	84.064 85.849 86.670 85.865	95.154 88.459 87.420 86.476	82.455	1.00 1.00 1.00	49.28
55	ATOM ATOM ATOM ATOM ATOM	8857 8858 8859 8860 8861	CB CG CD OE1	GLU E GLU E GLU E GLU E	3 379 3 379 3 379 3 379	86.427 87.385 88.484 88.025 87.059	85.632 86.628 87.413 88.775 88.832	78.660 81.284 81.956 82.405 83.215	1.00 1.00 1.00	34.07 35.34 39.50 43.86
60	ATOM ATOM ATOM ATOM ATOM	8862 8863 8864 8865 8866	N CA C	GLU E GLY E GLY E GLY E GLY E	380 380 380	88.608 84.556 83.705 83.334 83.083	89.777 86.651 85.747 84.470 83.450	81.927 79.251 78.507 79.280 78.654	1.00 1.00 1.00 1.00	46.28 33.33 32.76 31.95
C.F.	ATOM ATOM ATOM ATOM	8867 8868 8869 8870	N CA C	TYR B TYR B TYR B TYR B	381 381 381 381	83.316 82.882 81.604 81.552	84.498 83.340 83.722 84.769	80.613 81.381 82.133 82.750	1.00 1.00	32.76 29.75 28.76 28.78 29.82
65	ATOM ATOM ATOM	8874	CG CD1 CD2 CD2	TYR B TYR B TYR B	381 381 381	83.947 85.074 86.142 85.078	82.866 82.105 82.766 80.724	82.363 81.721 81.160 81.684	1.00 1.00 1.00	28.72 29.30 31.49
70	ATOM ATOM		CE1	ryr b ryr b		87.193 86.106	82.072 80.034	80.532 81.078	1.00	31.47

	ATOM	8877	CZ	TYR	В	381	87.163	80.732	80.492	1.00 32.82
	ATOM	8878	ОН			381	88.216	80.059	79.885	1.00 36.53
	ATOM	8879	N			382	80.580	82.874	82.059	1.00 27.19
	ATOM	8880	CA			382	79.314	83.098	82.722	1.00 26.71
5	ATOM	8881	C			382	79.386	82.934	84.261	1.00 25.48
_	ATOM	8882	ō			382	79.690	81.857	84.791	1.00 25.66
	ATOM	8883	ČВ	_		382	78.277	82.151	82.102	1.00 27.16
	ATOM	8884	CG	ARG			77.974	82.601	80.659	1.00 28.04
	ATOM	8885	CD	ARG			77.363	81.557	79.695	1.00 30.58
10	ATOM	8886	NE	ARG			77.567	82.097	78.355	1.00 30.30
10	ATOM	8887	CZ	ARG			76.882	83.109	77.849	1.00 31.62
	ATOM	8888		ARG			75.855	83.620	78.497	1.00 31.02
	ATOM	8889	NH2				77.211	83.594	76.673	1.00 32.85
	ATOM	8890	N	HIS			79.084	84.016	84.941	1.00 24.15
15	ATOM	8891	CA	HIS			79.165	84.137	86.401	1.00 23.61
13	ATOM	8892	C	HIS			77.978	84.910	86.989	1.00 23.83
	ATOM	8893	ŏ		В	383	77.300	85.645	86.276	1.00 23.03
	ATOM	8894	СВ		В	383	80.525	84.819	86.759	1.00 23.36
	ATOM	8895	CG	HIS		383	81.656	83.841	86.857	1.00 23.30
20	ATOM	8896		HIS		383	82.490	83.532	85.801	1.00 23.03
20	ATOM	8897		HIS		383	82.079	83.088	87.893	1.00 25.36
	ATOM	8898	CE1			383	83.371	82.630	86.186	1.00 23.99
	ATOM	8899	NE2	HIS		383	83.139	82.340	87.454	1.00 25.80
	ATOM	8900	N	ILE		384	77.739	84.763	88.302	1.00 25.28
25	ATOM	8901	CA	ILE		384	76.612	85.422	88.951	1.00 26.29
23	ATOM	8902	C	ILE		384	76.839	86.916	89.191	1.00 20.23
	ATOM	8903	Õ	ILE		384	77.830	87.297	89.825	1.00 27.05
	ATOM	8904	ČВ	ILE		384	76.295	84.719	90.285	1.00 26.60
	ATOM	8905	CG1			384	76.233	83.222	90.045	1.00 25.88
30	ATOM	8906	CG2	ILE			75.167	85.373	90.954	1.00 25.18
50	ATOM	8907		ILE			75.990	82.403	91.282	1.00 24.31
	ATOM	8908	N	CYS			75.912	87.738	88.701	1.00 29.31
	ATOM	8909	CA	CYS			75.907	89.180	88.884	1.00 25.31
	ATOM	8910	C	CYS		385	74.746	89.630	89.761	1.00 30.90
35	ATOM	8911	Ö			385	73.610	89.178	89.583	1.00 30.30
33	ATOM	8912	СB	CYS		385	75.741	89.914	87.552	1.00 32.52
	ATOM	8913	SG	CYS			77.023	91.169	87.259	1.00 32.32
	ATOM	8914	N	TYR			75.048	90.574		1.00 30.34
	ATOM	8915	CA	TYR		386	74.096	91.148	91.589	1.00 30.34
40	ATOM	8916	C	TYR		386	73.657	92.487	91.066	1.00 30.13
10	ATOM	8917	ŏ	TYR			74.472	93.316	90.795	1.00 30.40
	ATOM	8918	СВ	TYR			74.762	91.325	92.964	1.00 30.21
	ATOM	8919	CG	TYR			73.883	91.980	94.011	1.00 30.72
	ATOM	8920	CD1				72.621	91.474	94.301	1.00 29.66
45	ATOM	8921	CD2	TYR		386	74.329	93.076	94.732	1.00 32.09
10	ATOM	8922	CE1	TYR			71.802	92.084	95.267	1.00 33.09
	ATOM	8923	CE2				73.522	93.682	95.733	1.00 33.08
	ATOM	8924	CZ	TYR			72.276			1.00 31.44
	ATOM	8925	ОН	TYR			71.473	93.751	96.949	1.00 36.22
50	ATOM	8926	N	PHE			72.359	92.689	90.939	1.00 30.76
	ATOM	8927	CA	PHE			71.794	93.881	90.337	1.00 31.09
	ATOM	8928	C	PHE			70.891	94.524	91.384	1.00 32.31
	ATOM	8929	ō	PHE			70.170	93.836	92.091	1.00 30.31
	ATOM	8930	CB	PHE			70.906	93.514	89.127	1.00 31.28
55	ATOM	8931	CG	PHE			71.665	93.062	87.874	1.00 31.87
	ATOM	8932		PHE			71.999	91.738	87.675	1.00 30.46
	ATOM	8933		PHE			72.051	93.995	86.911	1.00 34.40
	ATOM	8934	CE1	PHE			72.683	91.335	86.539	1.00 33.89
	ATOM	8935		PHE			72.739	93.613	85.768	1.00 34.48
60	ATOM	8936	CZ	PHE			73.058	92.274	85.582	1.00 36.19
	ATOM	8937	N	GLN			70.896	95.845	91.468	1.00 34.06
	ATOM	8938	CA	GLN			69.942	96.521	92.340	1.00 35.90
	ATOM	8939	C	GLN			69.069	97.263	91.372	1.00 37.74
	ATOM	8940	ŏ	GLN			69.591	97.877	90.453	1.00 37.76
65	ATOM	8941	ČВ	GLN			70.654	97.415	93.358	1.00 37.70
	ATOM	8942	ČĞ	GLN			71.594	96.584	94.276	1.00 36.10
	ATOM	8943	CD	GLN			72.371	97.422	95.270	1.00 35.87
	ATOM	8944		GLN			72.861	98.479	94.926	1.00 38.43
	ATOM	8945	NE2	GLN			72.507	96.933	96.492	1.00 37.79
70	ATOM	8946	N	ILE			67.758	97.231	91.592	1.00 40.35
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	ATOM ATOM	8947 8948		ILE B		66.774 66.861				43.25 45.07
	ATOM ATOM	8949	_	ILE B		66.611	99.222	88.787	1.00	47.31
5		8950 8951		ILE B :	389 389	65.344 64.826				44.21
	ATOM	8952	CG	2 ILE B 3	389	64.392) 45.14) 44.71
	ATOM	8953		1 ILE B 3		63.959	95.453	91.453	1.00	47.44
	ATOM ATOM	8954 8955		ASP B 3		67.181 67.277	100.110			46.92
10		8956		ASP B 3			101.449 101.842			48.07 49.25
	ATOM	8957		ASP B 3	90	69.087	103.011	90.098		49.25
	ATOM ATOM	8958 8959		-		66.516	102.482	91.045	1.00	48.49
	ATOM	8960		1 ASP B 3	90	64.598	102.496 102.514	90.783 89.612		48.30
15	ATOM	8961	OD	2 ASP B 3	90	64.131	102.503	91.677		48.98
	ATOM ATOM	8962 8963		LYS B 3		69.642	100.852		1.00	50.15
	ATOM	8964		LYS B 3		71.075	101.102 100.336	89.821 88.592		50.80
••	ATOM	8965	0	LYS B 3	91	70.958	99.261	88.320		50.82 51.41
20	ATOM ATOM	8966 8967		LYS B 3		71.887	100.669	91.051	1.00	50.88
	ATOM	8968	CD	LYS B 3 LYS B 3		71.596	101.499 102.252	92.317 92.832		51.89
	MOTA	8969	CE	LYS B 3	91	72.503	103.218	93.957	1.00	53.68 55.27
25	ATOM ATOM	8970 8971	NZ	LYS B 3		73.674	104.105	94.333	1.00	57.04
23	ATOM	8972	N CA	LYS B 3 LYS B 3		72.448	100.865 100.359	87.867		51.42
	ATOM	8973	C	LYS B 3	92	73.714	99.176	86.536 86.410	1.00	51.86 51.31
	ATOM ATOM	8974 8975	0	LYS B 3	92	73.448	98.220	85.693	1.00	51.18
30	ATOM	8976	CB CG	LYS B 3		73.261	101.506 102.688	85.648		52.67
	ATOM	8977	CD	LYS B 3		75.348	102.688	86.392 85.871		54.96 58.49
	ATOM	8978	CE	LYS B 3	92	75.716	104.447	85.878		60.19
	ATOM ATOM	8979 8980	NZ N	LYS B 3			105.170	84.572	1.00	60.31
35	ATOM	8981	CA	ASP B 39		74.848 75.774	99.216 98.139	87.064 86.809		50.38
	ATOM	8982	C	ASP B 39	93	75.479	96.973	87.709		50.08 48.21
	ATOM	8983	0	ASP B 39		74.579	97.024	88.532		49.43
	ATOM ATOM	8984 8985	CB CG	ASP B 39		77.206 77.617	98.620	86.957		50.72
40	ATOM	8986	OD1	ASP B 39	93	77.555	99.543 99.116	85.820 84.628		53.43 55.71
	ATOM	8987		ASP B 39		77.999	100.714	86.034		57.39
	ATOM ATOM	8988 8989	N CA	CYS B 39		76.187	95.884	87.536	1.00	45.33
	ATOM	8990	C	CYS B 39	94	75.963 77.288	94.802 94.481	88.461 89.056		43.02 40.29
45	MOTA	8991	0	CYS B 39	4	78.308	95.025	88.650		38.33
	ATOM ATOM	8992 8993	CB	CYS B 39		75.347	93.604	87.766	1.00	43.53
	ATOM	8994	SG N	CYS B 39		76.360 77.250	92.904 93.629	86.459		44.49
	MOTA	8995	CA	THR B 39	5	78.437	93.246	90.060 90.763		37.49 35.54
50	ATOM	8996	C	THR B 39		78.599	91.760	90.638		33.54
	ATOM ATOM	8997 8998	O CB	THR B 39		77.741 78.290	90.995	91.057		32.26
	ATOM	8999		THR B 39	5	78.242	93.644 95.060	92.268 92.361		35.46 34.51
	ATOM	9000	CG2	THR B 39	5	79.534	93.247	93.102		35.50
55	ATOM ATOM	9001 9002	N	PHE B 39		79.705	91.356	90.053	1.00	32.02
	ATOM	9002	CA C	PHE B 39 PHE B 39		80.028 80.393	89.949 89.408	89.976 91.339		31.62
	ATOM	9004	Ö	PHE B 39	6	81.157	89.983	92.069	1.00 1.00	
60	ATOM	9005	CB	PHE B 39		81.158	89.704	88.994	1.00	
60	ATOM ATOM	9006 9007	CG CD1	PHE B 39 PHE B 39	6	80.707	89.754	87.577	1.00	32.92
	ATOM	9008	CD2	PHE B 39	6	79.940 81.012	88.718 90.852	87.049 86.773	1.00	
	ATOM	9009	CE1	PHE B 39	6	79.491	88.766	85.732	1.00	
65	ATOM	9010		PHE B 39		80.563	90.912	85.473	1.00	33.94
03	ATOM ATOM	9011 9012	CZ N	PHE B 39		79.795 79.857	89.853	84.950	1.00	
	ATOM	9013	CA	ILE B 39		79.857	88.249 87.618	91.632 92.911	1.00	30.00 28.98
	ATOM	9014	C	ILE B 39	7	80.719	86.311	92.760	1.00	
70	ATOM ATOM	9015	O CB	ILE B 39		81.147	85.707	93.756	1.00	26.77
, 0	11 OF	9016	СВ	ILE B 39	′	78.566	87.480	93.378	1.00	30.09

	ATOM ATOM ATOM	9017 9018 9019	CG1 CG2 CD1	ILE	В	397	78.255 78.181 77.145	88.618 86.088 89.355	94.308 93.850 93.736		30.11 33.13 34.11
	ATOM	9020	N			398	80.916	85.882	91.507		26.82
5	ATOM	9021	CA	THR			81.759	84.692	91.241	1.00	26.63
	MOTA	9022	С	THR			82.607	85.058	90.082		26.53
	ATOM	9023	0	THR			82.279	85.964	89.351		25.15
	MOTA	9024	CB	THR			80.958	83.405	90.855		26.34
	ATOM	9025	OG1	THR			80.066	83.700	89.776		24.02
10	ATOM	9026	CG2	THR LYS			80.114 83.699	82.910 84.354	91.966 89.906		24.85 27.52
	ATOM ATOM	9027 9028	N CA	LYS			84.562	84.650	88.796		29.60
	ATOM	9029	C	LYS			85.525	83.540	88.621		28.96
	ATOM	9030	ŏ	LYS			85.620	82.659	89.454		27.40
15	ATOM	9031	СB	LYS			85.331	85.973	89.004		30.65
	ATOM	9032	CG	LYS	В	399	86.196	85.968	90.241	1.00	33.69
	ATOM	9033	CD	LYS			87.538	86.536	89.932		39.54
	ATOM	9034	CE	LYS			87.562	88.053	89.776		41.78
••	ATOM	9035	NZ	LYS			88.942	88.504	89.306		45.54
20	MOTA	9036	N	GLY			86.219 87.209	83.587 82.608	87.494 87.186		28.97 29.71
	ATOM ATOM	9037 9038	CA C	GLY GLY			86.942	81.913	85.862		29.71
	ATOM	9039	Ö	GLY			85.961	82.201	85.158		30.25
	MOTA	9040	Ň	THR			87.839	81.000	85.550		29.97
25	ATOM	9041	CA	THR			87.836	80.234	84.296		31.55
	ATOM	9042	С	THR	В	401	86.956	79.005	84.392	1.00	29.87
	MOTA	9043	0	THR			87.419	77.881	84.282		30.82
	ATOM	9044	СВ	THR			89.266	79.725	84.038		31.58
20	MOTA	9045	OG1	THR			90.167	80.834	83.969		35.93
30	MOTA	9046	CG2	THR			89.362	79.179	82.687		35.92 28.95
	ATOM ATOM	9047 9048	N CA	TRP TRP	_	402 402	85.684 84.738	79.219 78.136	84.592 84.696		27.57
	ATOM	9049	CA	TRP			83.433	78.870	84.627		26.43
	ATOM	9050	Ö	TRP		402	83.435	80.082	84.519		24.58
35	ATOM	9051	ČВ	TRP		402	84.908	77.356	85991		27.62
	MOTA	9052	CG	TRP	В	402	85.024	78.201	87.275	1.00	29.73
	MOTA	9053	CD1				86.192	78.594	87.908		31.52
	MOTA	9054	CD2	TRP			83.953	78.686	88.102		30.78
40	ATOM	9055	NE1			402	85.906	79.278	89.065		31.48
40	ATOM	9056	CE2	TRP		402	84.548	79.365 78.599	89.215 88.039		32.72 28.88
	ATOM ATOM	9057 9058	CE3 CZ2	TRP TRP		402 402	82.564 83.797	79.979	90.216		30.83
	ATOM	9059	CZ3	TRP			81.810	79.196	89.044		30.58
	ATOM	9060	CH2	TRP			82.435	79.894	90.125		32.45
45	ATOM	9061	N	GLU			82.321	78.154	84.654	1.00	26.31
	ATOM	9062	CA	GLU			81.032	78.798	84.531	1.00	25.43
	MOTA	9063	С	GLU			79.993	78.330	85.506		24.97
	ATOM	9064	0	GLU			79.951	77.164			24.08
50	ATOM	9065	CB	GLU			80.476	78.571	83.141		24.99
50	MOTA MOTA	9066 9067	CG	GLU			81.355 80.550	79.047 79.358	82.020 80.756		26.01 30.67
	ATOM	9068	CD OF1	GLU			79.631	78.581	80.756		33.68
	ATOM	9069		GLU			80.805	80.383	80.077		32.90
	ATOM	9070	N	VAL			79.143	79.269	85.876		24.19
55	ATOM	9071°	CA	VAL			78.021	78.964	86.702		25.23
	ATOM	9072	С	VAL	В	404	77.000	78.456	85.747	1.00	25.03
	MOTA	9073	0	VAL	В	404	76.678	79.074	84.712		23.31
	ATOM	9074	CB	VAL			77.467	80.232	87.452		25.92
	ATOM	9075		VAL			76.106	79.958	88.025		27.06
60	ATOM	9076		VAL			78.470	80.712	88.550		23.98
	ATOM ATOM	9077 9078	N CA	ILE ILE			76.476 75.489	77.304 76.685	86.092 85.257		26.18 26.99
	ATOM	9078	CA	ILE			74.079	77.139	85.605		26.62
	ATOM	9080	0	ILE			73.263	77.366	84.720		25.39
65	ATOM	9081	СВ	ILE			75.670	75.240	85.340		27.77
	ATOM	9082		ILE			76.971	74.952	84.604		30.83
	ATOM	9083	CG2				74.449	74.493	84.696		29.84
	MOTA	9084		ILE			77.439	73.644	84.822	1.00	33.92
	ATOM	9085	N	GLY			73.803	77.312	86.884		25.76
70	ATOM	9086	CA	GLY	В	406	72.486	77.790	87.267	1.00	26.15

5	ATOM ATOM ATOM ATOM ATOM	9087 9088 9089 9090 9091	O N CA	GLY GLY ILE ILE	B B	407	72.456 73.205 71.615 71.286 70.081	77.6 79.2 79.6	98 61 74	88.716 89.554 88.981 90.347 90.832	1.0 1.0 1.0	0 26.05 0 26.77
10	ATOM ATOM ATOM ATOM ATOM	9092 9093 9094 9095 9096	CB CG1 CG2	ILE	B B B	407	68.983 70.943 72.205 70.365	78.9 81.1 81.9 81.4	33 45 53 91	90.237 90.378 90.101 91.655	1.0 1.0 1.0	0 27.55 0 26.48 0 26.38 0 27.27
	ATOM ATOM ATOM ATOM	9097 9098 9099 9100	N CA C	GLU	B B B	407 408 408 408 408	71.902 70.277 69.316 68.463 67.355	78.1 77.1 77.5	33 42 05	89.644 91.923 92.348 93.557 93.695	1.0 1.0 1.0	
15	ATOM ATOM ATOM ATOM ATOM	9101 9102 9103 9104 9105	CB CG CD OE1 OE2	GLU GLU GLU GLU	B B B	408 408 408	70.033 70.781 69.860 68.715 70.269	75.8 75.3 74.9 74.5	46 ! 23 ! 29 ! 32 !	92.615 91.405 90.275 90.478	1.00 1.00 1.00	0 28.28 0 30.97 0 31.77 0 32.78
20	ATOM ATOM ATOM ATOM ATOM	9106 9107 9108 9109 9110	N CA C O CB	ALA ALA ALA ALA	B B B	409 409 409 409	68.983 68.194 68.812 70.039	78.34 78.89 80.16	47. 9 95. 9 59. 9	39.156 94.438 95.507 96.106	1.00 1.00 1.00	27.82
25	ATOM ATOM ATOM ATOM	9111 9112 9113 9114	N CA C O	ALA LEU LEU LEU LEU	B B B	410 410 410 410	67.968 67.951 68.334 67.521 66.316	80.93 82.19 82.46	34 9 94 9 52 9	96.584 96.753 97.320 98.576 98.555	1.00 1.00 1.00	28.64 28.55 29.03 28.80 26.13
30	ATOM ATOM ATOM ATOM ATOM	9115 9116 9117 9118 9119		LEU LEU LEU THR	B B B	410 410 410	68.073 68.224 69.711 67.536 68.229	83.29 84.70 85.05 85.70 82.68)5 9 58 9 97 9	6.278 6.823 6.967 5.927 9.680	1.00 1.00 1.00	29.70 31.21 32.59 33.71 29.36
35	ATOM ATOM ATOM ATOM ATOM	9120 9121 9122 9123 9124	CA C O CB OG1	THR THR THR THR	B B	411	67.656 68.417 69.276 67.882 69.276	83.13 84.42 84.84 82.11	2 10 0 10 9 10 3 10	0.933 1.260 0.517 2.087 2.466	1.00 1.00 1.00	30.44 31.21 31.07 30.75 30.99
40	ATOM ATOM ATOM ATOM ATOM	9125 9126 9127 9128 9129	CG2 N CA C	THR SER SER SER SER	B A B A B A	411	67.613 68.166 68.879 70.348	80.69 85.01 86.23 86.02	6 10 5 10 0 10 7 10	1.653 2.408 2.750 3.168	1.00 1.00 1.00	31.01 32.99 33.86 33.76
45	ATOM ATOM ATOM ATOM	9130 9131 9132 9133	CB OG N CA	SER SER ASP ASP	B 4 B 4 B 4	412 412 413 413	71.138 68.136 68.298 70.711 72.094	86.97 86.94 86.25 84.82 84.54	9 10 1 10 0 10	3.098 3.855 5.064 3.609 4.037	1.00 1.00 1.00	35.07 34.08 37.09 33.55 33.66
50	ATOM ATOM ATOM ATOM ATOM	9134 9135 9136 9137 9138	O CB	ASP ASP ASP ASP	B 4 B 4	113 113 113	72.955 74.177 72.147 71.291 71.142	83.92 84.06 83.71 84.35 85.59	9 10 7 10 0 10	2.951 2.965 5.349 6.472 6.512	1.00 1.00 1.00 1.00	33.40 34.09 34.67 37.43
55	ATOM ATOM ATOM ATOM ATOM	9139 9140 9141 9142 9143	OD2 N CA C		B 4 B 4 B 4	113 114 114 114	70.682 72.315 73.023 72.379 71.164	83.67 83.24 82.44 82.40 82.52	7 10° 1 10° 2 10° 2 9°	7.314 2.004 1.042 9.639	1.00 1.00 1.00 1.00	35.18 41.17 32.74 32.44 31.27 29.95
60	ATOM ATOM ATOM ATOM ATOM	9144 9145 9146 9147 9148	CB CG CD1 CD2	TYR 1 TYR 1 TYR 1 TYR 1	3 4 3 4 3 4	114 114 114 114	73.061 73.550 74.871 72.691 75.319	81.010 80.834 81.095 80.385 80.908	0 101 4 102 5 103 9 103	1.548 2.967 3.311 3.964	1.00 1.00 1.00 1.00	33.10 37.63 43.56 42.38 45.87
65	ATOM ATOM ATOM ATOM ATOM	9149 9150 9151 9152 9153	CE2 CZ COH COH CON I	TYR I TYR I TYR I LEU I LEU I	3 4 3 4 3 4 3 4	14 14 14	73.130 74.442 74.876 73.237 72.847	80.234 80.506 80.344 82.251 81.988	1 105 5 105 1 106 1 98	5.262 5.570 5.861 3.615	1.00 1.00 1.00 1.00	45.10 45.30 51.32 29.76 28.70
70	ATOM ATOM ATOM	9154 9155 9156	0 1	PEA E PEA E PEA E	3 4	15	73.486 74.708 73.371	80.654 80.467 83.056	96	.880 .041 .271	1.00	28.09 27.98 28.13

	ATOM ATOM ATOM	9157 9158 9159		LEU LEU	В		72.962 72.755 73.952	82.857 84.190 81.961	94.815 94.108 94.065		29.69 29.73 30.10
5	ATOM ATOM ATOM	9160 9161 9162	N CA C	TYR TYR	B B	416 416 416	72.675 73.186 73.166	79.708 78.391 78.226	96.432 96.098 94.565	1.00 1.00	
	ATOM ATOM ATOM	9163 9164 9165	O CB CG	TYR TYR	B B	416 416 416	72.160 72.308 72.240	78.527 77.281 77.193	93.927 96.697 98.173	1.00 1.00	28.15
10	ATOM ATOM ATOM	9166 9167 9168	CD2 CE1	TYR	B B	416 416	71.371 72.953 71.247		98.876 98.868 100.196	1.00 1.00	27.63 28.81 28.41
15	ATOM ATOM ATOM ATOM	9169 9170 9171 9172	CE2 CZ OH N	TYR TYR	B B	416 416 416 417	72.822 71.970 71.763 74.250	76.176 77.042 77.015 77.723	100.242 100.887 102.225 94.003	1.00 1.00	31.88 30.74 27.12 24.99
	ATOM ATOM ATOM	9173 9174 9175	CA C O	TYR	B B	417 417	74.373 75.128 75.848	77.573 76.325 75.757	92.573 92.181 92.985	1.00 1.00	25.31 24.04 23.73
20	ATOM ATOM ATOM	9176 9177 9178	CB CG CD1	TYR TYR	B B		75.065 76.537 76.976	78.809 78.928 79.616	91.972 92.293 93.428	1.00	25.15 28.08 27.99
25	ATOM ATOM ATOM ATOM	9179 9180 9181 9182		TYR TYR TYR TYR	B B	417 417	77.500 78.331 78.852 79.253	78.329 79.734 78.418 79.143	91.491 93.718 91.811 92.915	1.00 1.00	28.55 27.43 29.29 28.63
	ATOM ATOM ATOM	9183 9184 9185	OH N CA	TYR ILE ILE	B B	417 418	80.606 74.960 75.687	79.212 75.903 74.766	93.242 90.932 90.395	1.00	29.92 22.92 22.89
30	ATOM ATOM ATOM	9186 9187 9188	C O CB	ILE ILE ILE	B B	418 418	76.734 76.488 74.727	75.268 76.179 73.795	89.427 88.668 89.704	1.00 1.00 1.00	22.06 21.82 24.28
35	ATOM ATOM ATOM	9189 9190 9191 9192		ILE ILE	B B	418 418	73.965 75.475 72.754 77.921	73.011 72.742 72.473 74.707	90.762 88.818 90.209 89.459	1.00 1.00	26.51 23.28 26.35 22.69
·	ATOM ATOM ATOM ATOM	9193 9194 9195	N CA C O	SER SER SER	B B	419 419	78.984 79.863 79.835	75.110 73.981 72.928	88.501 88.105 88.740	1.00	22.54 22.43 22.38
40	ATOM ATOM ATOM	9196 9197 9198	CB OG N	SER SER ASN	B B B	419 419 420	79.892 80.960 80.682	76.217 75.726 74.209	89.080 89.913 87.078	1.00 1.00 1.00	23.04 22.13 22.56
45	ATOM ATOM ATOM	9199 9200 9201	CA C O	ASN ASN	B B	420 420	81.700 83.064 84.080	73.236 73.570 73.076	86.735 87.316 86.795	1.00	23.33 24.36 23.91 23.30
	ATOM ATOM ATOM ATOM	9202 9203 9204 9205		ASN ASN ASN	B B	420 420	81.859 82.003 81.738 82.358	72.970 74.234 74.231 75.321	85.212 84.387 83.187 85.026	1.00	23.65 25.64 24.56
50	ATOM ATOM ATOM	9206 9207 9208	N CA C	GLU GLU GLU	B B	421 421	83.104 84.396 85.244	74.307 74.668 73.495	88.432 88.992 89.362	$1.00 \\ 1.00$	25.65 26.66 26.87
55	ATOM ATOM ATOM	9209 9210 9211	O CB CG	GLU GLU GLU	B B B	421 421 421	86.443 84.304 85.672	73.530 75.596 76.069	89.134 90.251 90.692	1.00 1.00	28.68 27.29 28.18
	ATOM ATOM ATOM	9212 9213 9214	OE2	GLU GLU	B B	421 421	85.657 84.593 86.743	77.091 77.354 77.642	91.819 92.391 92.101	1.00 1.00	30.20 28.33 30.05
60	ATOM ATOM ATOM ATOM	9215 9216 9217 9218	N CA C	TYR TYR TYR TYR	B B	422 422	84.668 85.499 86.528 86.189	72.470 71.428 70.779 70.226	89.966 90.558 89.621 88.558	1.00	28.24 29.25 30.07 27.85
65	ATOM ATOM ATOM	9219 9220 9221	CB CG	TYR TYR TYR	B B	422 422	84.630 85.346 86.083	70.374 69.559 70.174	91.187 92.200 93.237	1.00 1.00 1.00	29.87 33.87 35.94
	ATOM ATOM	9222 9223 9224	CE1 CE2	TYR TYR TYR	B B	422 422	85.310 86.749 85.980	68.161 69.415 67.393	92.147 94.164 93.088	1.00 1.00	35.90 35.72 34.40
70	ATOM ATOM	9225 9226	CZ OH	TYR TYR			86.674 87.336	68.013 67.228	94.091 95.014		37.30 39.63

ATOM

N

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9227
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GLY B 427
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GLY B 428
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76.286
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92.508
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                         ASN B 430
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77.276
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                         ASN B
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75.524
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72.713
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                         LEU
                              B 431
                                                    71.849
                                                                       1.00 21.87
                                                              96.637
     MOTA
             9290
                                                    74.679
75.589
                    N
                         TYR
                              В
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                                                              95.031
                                                                       1.00 25.52
65
    ATOM
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                    CA
                             В
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                         TYR
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                    С
                         TYR
                             B 432
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                                                    76.564
                                                              96.670
                                                                       1.00 26.29
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                             B 432
                         TYR
                                           75.879
                                                    76.822
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    ATOM
             9294
                    CB
                         TYR
                              В
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                                           79.083
                                                    76.397
                                                              95.231
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    ATOM
             9295
                                           80.157
                    CG
                         TYR B 432
                                                    75.564
                                                              94.491
                                                                       1.00 26.70
70
    MOTA
             9296
                    CD1 TYR B 432
                                           79.870
                                                    74.928
                                                              93.298
                                                                       1.00 25.29
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	ATOM	9297	CD2	TYR	B 432	81.461	75.459	94.981	1.00	29.33
	ATOM	9298	CE1				74.172	92.643	1.00	26.84
	ATOM	9299	CE2			82.442	74.723	94.302	1.00	28.11
	ATOM	9300	CZ		B 432	82.103	74.074		1.00	
_				_						
5	ATOM	9301	OH	TYR		83.042	73.324	92.479	1.00	
	ATOM	9302	N	LYS :	в 433	77.586	77.137	97.715	1.00	26.07
	ATOM	9303	CA	LYS :	B 433	76.914	78.002	98.601	1.00	28.02
	ATOM	9304	С	LYS		77.777	79.265	98.873	1.00	
	ATOM	9305	ŏ	LYS		78.951	79.179	99.267		
									1.00	
10	ATOM	9306	CB	LYS		76.702	77.185	99.868	1.00	
	ATOM	9307	CG	LYS	3 433	75.957	77.846	100.956	1.00	31.09
	ATOM	9308	CD	LYS	3 433	76.123	77.047	102.240	1.00	34.56
	ATOM	9309	CE	LYS		75.152				36.16
				_						
	MOTA	9310	NZ	LYS		75.234		104.562		34.35
15	ATOM	9311	N	ILE !		77.195	80.431	98.653	1.00	
	ATOM	9312	CA	ILE 1	3 434	77.888	81.680	98.925	1.00	28.10
	ATOM	9313	С	ILE I	3 434	77.183	82.400	100.044	1.00	27.39
	ATOM	9314	ŏ	ILE		75.950	82.589	99.989	1.00	
				ILE		77.829				
	ATOM	9315	СВ				82.611	97.742	1.00	
20	ATOM	9316	CG1			78.135	81.917	96.436	1.00	28.81
	ATOM	9317	· CG2	ILE 1	3 434	78.818	83.742	97.905	1.00	29.92
	ATOM	9318	CD1	ILE I	3 434	77.749	82.790	95.262	1.00	29.33
	ATOM	9319	N	GLN I		77.955		101.039		27.61
	ATOM	9320	CA	GLN I		77.449	83.693	102.094		28.32
25	MOTA	9321	С	GLN I		77.384	85.069	101.533	1.00	27.86
	ATOM	9322	0	GLN F	3 435	78.388	85.589	101.142	1.00	28.87
	ATOM	9323	CB	GLN F	3 435	78.415	83.792	103.274	1.00	29.60
	ATOM	9324	CG	GLN I		78.708	82.549	103.997		32.31
	ATOM	9325	CD	GLN E		79.361	82.786	105.354		39.38
30	ATOM	9326	OE1			78.832	83.531	106.192	1.00	40.29
	ATOM	9327	NE2	GLN E	3 435	80.488	82.107	105.592	1.00	35.81
	ATOM	9328	N	LEU E		76.224	85.688	101.526	1.00	28.49
	ATOM	9329	CA	LEU E		76.063	86.996	100.920		28.61
	ATOM	9330	C	LEU E		76.790	88.146	101.680		29.22
35	ATOM	9331	0	LEU E	3 436	76.972	89.207	101.126		28.54
	ATOM	9332	CB	LEU E	3 436	74.554	87.255	100.718	1.00	28.45
	ATOM	9333	CG	LEU E	436	73.897	86.104	99.912	1.00	28.99
	ATOM	9334		LEU E		72.411	86.225	99.772		29.93
	MOTA	9335		LEU E		74.557	86.016	98.503		31.60
40	ATOM	9336	N	SER E	3 437	77.220	87.914	102.916	1.00	29.84
	ATOM	9337	CA	SER E	437	77.941	88.904	103.708	1.00	31.25
	MOTA	9338	С	SER E	437	79.450	89.025	103.325	1.00	31.20
	ATOM	9339	ō	SER E		80.142	89.931	103.785		33.20
	ATOM	9340	CB	SER E		77.738	88.593	105.209		31.10
45	ATOM	9341	OG	SER E		78.718	87.662	105.727		33.45
	ATOM	9342	N	ASP E	438	79.925	88.093	102.480	1.00	31.28
	ATOM	9343	CA	ASP E	438	81.309	88.002	102.006	1.00	31.22
	ATOM	9344	C	ASP E		81.383		100.866		31.12
				ASE L	420					
	ATOM	9345	0	ASP E		81.469		101.101		29.30
50	ATOM	9346	CB	ASP E		82.279	87.641	103.134		31.63
	ATOM	9347	CG	ASP E	438	83.732	87.507	102.655	1.00	34.50
	ATOM	9348	OD1	ASP E		84.011	87.584	101.430		37.97
	ATOM	9349		ASP E		84.675	87.335	103.457		40.92
	MOTA	9350	N	TYR E		81.388	87.432	99.638		31.76
55	MOTA	9351	CA	TYR E	439	81.363	86.596	98.449	1.00	32.36
	ATOM	9352	С	TYR E	439	82.532	85.657	98.377	1.00	33.28
	ATOM	9353	Ō	TYR E		82.527	84.743	97.563		33.53
	ATOM	9354	ČВ	TYR E		81.310	87.472	97.182		32.45
	ATOM	9355	CG	TYR E		80.147	88.444	97.151		29.88
60	ATOM	9356	CD1	TYR E	439	78.929	88.090	97.671	1.00	31.80
	ATOM	9357	CD2	TYR E	439	80.273	89.703	96.593		29.37
	ATOM	9358	CE1	TYR E		77.842	88.963	97.670		31.92
	MOTA	9359	CE2	TYR B		79.192	90.610	96.599		30.27
	ATOM	9360	CZ	TYR E		77.980	90.205	97.126		32.14
65	ATOM	9361	OH	TYR E	439	76.891	91.018	97.115	1.00	32.51
	ATOM	9362	N	THR B		83.535	85.827	99.237		33.58
	ATOM	9363	CA	THR B		84.728	84.991	99.124		33.41
	MOTA	9364	C	THR B		84.504	83.761	99.940		33.90
	MOTA	9365	0	THR B	440	85.247	82.801	99.862		33.02
70	MOTA	9366	CB	THR B	440	85.969	85.708	99.642	1.00	34.51

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                                                      86.038 101.022
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       ATOM
               9368
                       CG2
                           THR B 440
                                             86.162
                                                      87.058
                                                               98.952
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       ATOM
               9369
                      N
                           LYS
                               B 441
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               9370
                      CA
                           LYS B 441
                                             83.162
                                                      82.649
                                                              101.570
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                                                                               35.47
       ATOM
               9371
                      C
                           LYS B 441
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               9372
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                           LYS
                               B 441
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                                                      81.992 100.765
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                      CG
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9377
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82.836
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97.796
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               9383
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      ATOM
               9384
                      CG2 VAL B 442
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73.317
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94.730
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45
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82.850
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67.903
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96.379
95.723
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              9413
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                         CYS B 447
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                         CYS B 447
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86.776
86.858
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60
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                    OE2
                         GLU B 448
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98.715
                                                    67.372
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     ATOM
             9427
                         LEU B 449
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                    Ŋ
                                           81.370
                                                                             33.47
                                                                       1.00
             9428
     MOTA
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80.726
80.551
                         LEU B 449
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     ATOM
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                    C
                         LEU B 449
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                    CA
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	ATOM ATOM ATOM	9437 9438 9439	C O CB	ASN ASN	B 450 B 450 B 450	82.036 81.498 79.911	60.852 60.567 60.067	96.017 94.969 96.990	1.00 34.66 1.00 34.27 1.00 35.97
5	ATOM ATOM ATOM ATOM	9440 9441 9442 9443	CG OD1 ND2 N	ASN ASN	B 450 B 450 B 450 B 451	79.281 79.803 78.079 83.285	59.263 58.213 59.697 61.294	98.097 98.492 98.546 96.085	1.00 40.57 1.00 44.98 1.00 42.91 1.00 35.39
10	ATOM ATOM ATOM ATOM	9444 9445 9446 9447	CA C O CB	PRO PRO	B 451 B 451 B 451 B 451	84.036 84.399 84.689 85.347	61.820 60.928 61.437 62.340	94.919 93.726 92.662 95.529	1.00 34.83 1.00 35.41 1.00 34.70 1.00 34.92
	ATOM ATOM ATOM	9448 9449 9450	CG CD N	PRO PRO	B 451 B 451 B 452	85.310 84.081 84.468	62.005 61.259 59.625	97.016 97.337 93.899	1.00 36.21 1.00 35.15 1.00 36.27
15	ATOM ATOM ATOM ATOM	9451 9452 9453 9454	CA C O CB	GLU GLU	B 452 B 452 B 452 B 452	84.771 83.504 83.536 85.459	58.782 58.377 58.042 57.517	92.769 92.047 90.871 93.226	1.00 36.68 1.00 35.32 1.00 35.61 1.00 37.91
20	ATOM ATOM ATOM	9455 9456 9457	CG CD OE1	GLU GLU	B 452 B 452 B 452	86.958 87.396 87.352	57.644 57.480 56.315	93.324 94.747 95.221	1.00 41.25 1.00 46.23 1.00 50.42
25	ATOM ATOM ATOM ATOM	9458 9459 9460 9461	OE2 N CA C	ARG ARG	B 452 B 453 B 453 B 453	87.757 82.399 81.134 80.325	58.506 58.368 57.969 59.160	95.379 92.780 92.228 91.742	1.00 48.73 1.00 33.86 1.00 32.45 1.00 31.92
	ATOM ATOM ATOM	9462 9463 9464	O CB CG	ARG ARG ARG	B 453 B 453 B 453	79.527 80.330 79.002	59.049 57.222 56.646	90.813 93.275 92.768	1.00 30.67 1.00 32.79 1.00 31.10
30	ATOM ATOM ATOM ATOM	9465 9466 9467 9468	CD NE CZ NH1	ARG	B 453 B 453 B 453 B 453	78.183 76.827 76.050 76.521	56.114 55.806 54.974 54.366	93.884 93.497 94.169 95.252	1.00 32.75 1.00 34.45 1.00 33.89 1.00 31.33
35	ATOM ATOM ATOM	9469 9470 9471	NH2 N CA	ARG CYS CYS	B 453 B 454 B 454	74.803 80.537 79.628	54.737 60.311 61.416	93.766 92.348 92.077	1.00 31.42 1.00 30.98 1.00 30.23
	ATOM ATOM ATOM ATOM	9472 9473 9474 9475	C O CB SG	CYS CYS	B 454 B 454 B 454 B 454	80.330 80.968 78.722 77.582	62.698 / 63.299 61.596 60.243	91.739 92.581 93.271 93.475	1.00 28.75 1.00 28.32 1.00 30.58 1.00 30.80
40	ATOM ATOM ATOM	9476 9477 9478	N CA C	GLN GLN GLN	B 455 B 455 B 455	80.198 80.859 79.901	63.100 64.284 65.140	90.479 89.977 89.143	1.00 27.50 1.00 26.27 1.00 25.48
45	ATOM ATOM ATOM ATOM	9479 9480 9481 9482	O CB CG CD	GLN	B 455 B 455 B 455 B 455	80.327 82.092 83.283 84.294	66.147 63.894 63.322 62.520	88.624 89.132 89.864 88.937	1.00 25.25 1.00 25.42 1.00 27.34 1.00 32.33
	ATOM ATOM ATOM	9483 9484 9485	OE1 NE2 N	GLN TYR	B 455 B 455 B 456	84.123 85.320 78.637	62.440 61.948 64.728	87.732 89.535 89.008	1.00 32.86 1.00 31.75 1.00 25.74
50	ATOM ATOM ATOM ATOM	9486 9487 9488 9489	CA C O CB	TYR TYR	B 456 B 456 B 456 B 456	77.616 76.305 75.471 77.336	65.451 65.566 64.642 64.745	88.214 89.017 89.062 86.880	1.00 26.19 1.00 26.13 1.00 26.14 1.00 26.83
55	ATOM ATOM ATOM	9490 9491 9492	CG CD1 CD2	TYR TYR TYR	B 456 B 456 B 456	76.775 75.408 77.613	65.604 65.856 66.155	85.763 85.647 84.811	1.00 24.10 1.00 25.09 1.00 25.81
60	ATOM ATOM ATOM ATOM	9493 9494 9495 9496	CE1 CE2 CZ OH	TYR TYR	B 456 B 456 B 456 B 456	74.884 77.120 75.759 75.326	66.645 66.931 67.171 67.971	84.564 83.752 83.632 82.582	1.00 23.20 1.00 22.75 1.00 24.21 1.00 23.14
00	ATOM ATOM ATOM	9497 9498 9499	N CA C	TYR TYR	B 457 B 457 B 457	76.126 74.969 73.966	66.699 66.874 67.883	89.668 90.535 89.981	1.00 25.26 1.00 24.93 1.00 25.41
65	ATOM ATOM ATOM ATOM	9500 9501 9502 9503	O CB CG CD1	TYR	B 457 B 457 B 457 B 457	74.353 75.416 76.131 75.407	68.823 67.413 66.426 65.643	89.273 91.887 92.804 93.682	1.00 24.40 1.00 25.11 1.00 24.76 1.00 26.61
70	ATOM ATOM ATOM	9504 9505 9506	CD2 CE1	TYR TYR	B 457 B 457 B 457	77.505 76.013 78.142	66.326 64.761 65.414	92.832 94.544 93.694	1.00 23.91 1.00 25.28 1.00 26.22

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ATOM
                9507
                       CZ
                            TYR B 457
                                              77.378
                                                       64.647
                                                                 94.538
                                                                           1.00 25.74
       MOTA
                9508
                       OH
                            TYR B 457
                                              77.941
                                                       63.748
                                                                 95.387
                                                                           1.00 29.90
       ATOM
                9509
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                            SER B 458
                                                       67.629
                                              72.684
                                                                 90.267
                                                                           1.00 25.31
       MOTA
                9510
                       CA
                            SER B 458
                                             71.622
                                                       68.618
                                                                 90.197
                                                                           1.00 26.57
       ATOM
                9511
                       С
                            SER B 458
                                             70.940
                                                       68.599
                                                                 91.598
                                                                           1.00 26.57
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                9512
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                            SER B 458
                                             71.214
                                                       67.736
                                                                 92.401
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                9514
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                            SER B 458
                                                       67.072
                                                                 89.530
                                                                           1.00 30.73
       ATOM
                9515
                       N
                            VAL B 459
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                                                       69.541
                                                                 91.890
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                                                                                 27.82
  10
       ATOM
                9516
                       CA
                           VAL B 459
                                             69.487
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                                                                 93.224
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       ATOM
                9517
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67.659
                                                       70.172
70.785
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                           VAL B 459
                                                                 93.170
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       MOTA
                9518
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                           VAL B 459
                                                                 92.199
                                                                          1.00 25.23
               9519
       ATOM
                       СВ
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                           VAL B 459
                                             70.333
                                                                 94.044
                                                                          1.00 28.32
                           VAL B 459
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                                                       72.074
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                                                                          1.00 28.21
  15
               9521
       ATOM
                                             69.956
67.335
                       CG2
                           VAL B 459
                                                       70.722
                                                                95.464
94.266
                                                                          1.00 28.98
       ATOM
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                           SER B 460
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                                                       69.956
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                      CA
                           SER B 460
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                                                                          1.00 28.37
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               9524
       MOTA
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65.780
                           SER B 460
                                                       70.855
                                                                95.861
                                                                          1.00
                                                                                28.75
               9525
       MOTA
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                           SER B 460
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                                                                          1.00 29.69
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69.512
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                      OG
                           SER B 460
                                             63.716
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                                                                                29.79
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               9528
                      N
                           PHE B 461
                                             65.597
                                                       72.150
                                                                96.096
                                                                          1.00
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64.022
                      CA
                           PHE B 461
                                                      72.713
                                                                97.416
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                      С
                           PHE B 461
                                                                97.845
97.053
                                                       72.821
                                                                          1.00 29.45
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                           PHE B 461
                                             63.196
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                                                                          1.00
                                                                                28.41
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               9532
                      CB
                           PHE B 461
                                                                97.446
                                             66.075
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                                                                          1.00
                                                                                28.68
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               9533
                                            67.584
68.236
                      CG
                           PHE B 461
                                                      74.176
                                                                97.514
                                                                          1.00 28.23
      ATOM
               9534
                      CD1 PHE B 461
                                                      74.124
74.261
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      ATOM
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                      CD2 PHE B 461
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                      CE1 PHE B 461
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                      CE2
                           PHE B 461
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                      CA
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62.755
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                      CA
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76.615 100.104
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60.724
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77.006 101.148
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                         GLU B 464
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67.347
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77.210 100.607
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                         ALA B 465
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                         LYS B 466
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                         LYS B 466
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	ATOM ATOM	9577 9578	N CA	TYR	В	467 467	65.747 66.300		103.215 102.860	1.00	31.59 30.73
	ATOM	9579	C			467	66.474		101.358		29.96
_	ATOM	9580	0			467	65.889		100.604		28.87
5	ATOM ATOM	9581 9582	CB CG			467 467	65.382 65.066		103.319 104.796		31.25 30.99
	ATOM	9583	CD1			467	63.998		104.790		33.27
	ATOM	9584	CD2			467	65.800		105.673		30.15
	ATOM	9585	CE1			467	63.686		106.688		33.81
10	ATOM	9586	CE2	TYR	В	467	65.500	69.262	107.043	1.00	32.44
	MOTA	9587	CZ			467	64.443		107.533		32.21
	ATOM	9588	ОН			467	64.127		108.883		32.73
	ATOM	9589	N			468	67.287		100.940		29.46
15	ATOM	9590 9591	CA			468 468	67.547 67.794	69.847 68.381	99.537 99.253		28.49
13	ATOM ATOM	9592	C O			468	68.358		100.095		28.61 28.77
	ATOM	9593	СВ			468	68.707	70.709	99.012	1.00	27.78
	ATOM	9594	CG			468	70.088	70.640	99.691	1.00	
	ATOM	9595	CD1			468	70.398		100.759		28.76
20	MOTA	9596	CD2			468	71.101	69.816	99.211		28.66
	MOTA	9597	CE1			468	71.641		101.357		28.54
	ATOM	9598	CE2			468	72.367	69.793	99.805		28.13
	ATOM	9599	CZ			468	72.617	70.623	100.880		27.70
25	ATOM ATOM	9600 9601	N OH			468 469	73.837 67.333	70.630 67.947	101.527 98.078		27.01 28.39
23	ATOM	9602	CA			469	67.655	66.620	97.552		27.88
	ATOM	9603	C			469	68.787	66.762	96.570		27.66
	ATOM	9604	ō			469	68.701	67.579	95.670		26.59
	ATOM	9605	CB	GLN	В	469	66.480	66.001	96.776		28.62
30	MOTA	9606	CG			469	66.748	64.572	96.227		26.39
	ATOM	9607	CD			469	65.749	64.143	95.130		28.98
	MOTA	9608		GLN			65.374	64.939	94.301		31.48
	ATOM ATOM	9609 9610	NEZ N	GLN LEU			65.268 69.840	62.896 65.968	95.193 96.730		29.61 27.61
35	ATOM	9611	CA	LEU			70.898	65.928	95.754		28.28
	ATOM	9612	C	LEU			70.746	64.731	94.849		28.23
	ATOM	9613	ō	LEU			70.341	63.656	95.304		27.32
	ATOM	9614	CB	LEU	В	470	72.279	65.892	96.388		27.67
	ATOM	9615	CG	LEU			72.785	67.229	96.904		30.41
40	ATOM	9616	CD1	LEU			74.044	66.988	97.626		28.59
	ATOM ATOM	9617 9618		LEU			72.985	68.289 64.950	95.801		31.31
	ATOM	9619	N CA	ARG ARG			71.059 70.967	63.945	93.568 92.522		28.24 29.03
	ATOM	9620	C.	ARG			72.295	63.882	91.765		29.35
45	ATOM	9621	ŏ	ARG			72.635	64.753	90.965	1.00	
	MOTA	9622	CB	ARG	В	471	69.859	64.231	91.485		30.47
	MOTA	9623	CG	ARG			70.105	63.401	90.148		35.53
	ATOM	9624	CD	ARG	_		68.872	63.172	89.177		42.75
50	ATOM	9625	NE	ARG			68.849	64.130	88.078		47.16
50	ATOM ATOM	9626 9627	CZ NH1	ARG ARG			67.781 66.603	64.435 63.840	87.344 87.555		51.84 52.12
	ATOM	9628		ARG			67.905	65.353	86.389		51.86
	ATOM	9629	N	CYS			73.039	62.843	92.071		29.45
	ATOM	9630	CA	CYS			74.273	62.560	91.411		30.96
5 5	MOTA	9631	С	CYS			73.955	61.712	90.186	1.00	29.94
	ATOM	9632	0	CYS			73.263	60.743	90.315		29.73
	ATOM	9633	CB	CYS			75.137	61.782	92.412		31.75
	ATOM	9634	SG	CYS			76.340	60.578	91.768		36.58
60	ATOM ATOM	9635	N	SER SER			74.462 74.212	62.081	89.014		29.26 29.27
60	ATOM	9636 9637	CA C	SER			75.397	61.325 60.566	87.795 87.258		27.53
	ATOM	9638	0	SER			75.282	59.961	86.221		27.50
	ATOM	9639	ČВ	SER			73.731	62.245	86.684		28.76
	ATOM	9640	OG	SER			72.382	62.487	86.896		32.10
65	ATOM	9641	N	GLY			76.525	60.578	87.943		26.50
	ATOM	9642	CA	GLY			77.666	59.806	87.503		25.47
	ATOM	9643	C	GLY			78.932	60.365	88.098		25.87
	ATOM	9644	0	GLY			78.846	61.403	88.770		25.00
70	ATOM	9645	N	PRO			80.108	59.796	87.778		26.49
70	MOTA	9646	CA	PRO	B	4/3	80.259	58.688	86.820	T.00	26.73

	MOTA MOTA MOTA MOTA	9647 9648 9649 9650	O PR	O B 475 O B 475 O B 475 O B 475	79.769 79.668 81.782	56.558 58.574	87.280 86.405 86.624	1.00 26.57 1.00 27.70
5		9651 9652 9653 9654	CD PR N GL CA GL	O B 475 O B 475 Y B 476 Y B 476 Y B 476	82.343 81.427 79.483 78.979 77.468	60.304 57.177 55.898	87.911 88.212 88.578 89.060	1.00 26.62 1.00 27.70 1.00 26.91
10	ATOM	9655 9656 9657 9658	O GL N LE CA LE	Y B 476 U B 477 U B 477 U B 477	76.858 76.854 75.414 74.786	56.716	88.895 88.201 89.489 89.460 90.179	1.00 27.17 1.00 26.20 1.00 27.44 1.00 29.14 1.00 29.25
15	ATOM ATOM ATOM	9659 9660 9661 9662	O LE CB LE CG LE CD1 LE	U B 477 U B 477 U B 477 U B 477	75.281 74.986 75.705 75.080	56.352 53.436 52.213 50.971	91.229 90.149 89.586 90.149	1.00 29.25 1.00 28.98 1.00 29.87 1.00 33.15 1.00 35.05
20	ATOM ATOM ATOM ATOM ATOM	9663 9664 9665 9666 9667	N PRO CA PRO C : PRO	J B 477 D B 478 D B 478 D B 478 D B 478	75.645 73.711 72.984 72.717	52.212 56.434 57.552 57.345	88.035 89.610 90.226 91.708	1.00 35.43 1.00 29.49 1.00 28.80 1.00 28.27
25	ATOM ATOM ATOM ATOM	9668 9669 9670 9671	CB PRO	D B 478 D B 478 D B 478 D B 478 J B 479	72.384 71.673 72.099 73.115 72.806	56.230 57.577 57.117 56.029 58.431	92.132 89.432 88.030 88.325 92.462	1.00 28.59 1.00 28.93 1.00 29.83 1.00 29.62 1.00 27.47
	ATOM ATOM ATOM ATOM	9672 9673 9674 9675	CA LET C LET C LET CB LET	J B 479 J B 479 J B 479 J B 479	72.659 71.794 72.108 74.048	58.444 59.627 60.779 58.628	93.903 94.339 94.071 94.544	1.00 27.62
30	ATOM ATOM ATOM ATOM	9676 9677 9678 9679	CD1 LEU CD2 LEU N TYF	В 479 В В 480	74.281 75.361 73.037 70.711	57.974 58.642 57.890 59.355	95.893 96.719 96.694 95.023	1.00 31.83 1.00 33.40 1.00 33.81 1.00 26.74
35	ATOM ATOM ATOM ATOM ATOM	9680 9681 9682 9683 9684	C TYF O TYF CB TYF	B 480 B 480 B 480 B 480 B 480	69.848 69.858 69.579 68.423	60.420 60.524 59.543 60.190	95.438 96.971 97.693 94.938	1.00 27.84 1.00 27.91 1.00 28.32 1.00 28.47
40	ATOM ATOM ATOM ATOM	9685 9686 9687 9688	CD1 TYR CD2 TYR CE1 TYR	В 480 В 480	68.258 68.722 67.591 68.538 67.423	60.043 58.922 61.015 58.785 60.911	93.408 92.727 92.679 91.304 91.295	1.00 28.87 1.00 29.58 1.00 30.14 1.00 29.30 1.00 31.04
45	ATOM ATOM ATOM ATOM ATOM	9689 9690 9691 9692 9693	CZ TYR OH TYR N THR CA THR	B 480 B 480 B 481 B 481 B 481	67.909 67.703 70.133 70.252	59.797 59.712 61.717 61.928	90.613 89.257 97.460 98.888	1.00 30.37 1.00 32.11 1.00 27.62 1.00 28.14
50	ATOM ATOM ATOM ATOM	9694 9695 9696 9697	O THR	B 481 B 481 B 481	69.454 69.095 71.713 72.253 72.567	63.124 64.012 62.164 63.151 60.907	99.348 98.546 99.225 98.338 98.947	1.00 28.12 1.00 26.65 1.00 28.73 1.00 29.12 1.00 28.66
55	ATOM ATOM ATOM ATOM ATOM	9698 9699 9700 9701 9702	CA LEU C LEU C LEU CB LEU	B 482 B 482 B 482 B 482 B 482	69.180 68.458 69.356 70.196 67.177	63.137 1 64.229 1 64.914 1 64.291 1 63.752 1	L00.649 L01.282 L02.280 L02.924	1.00 28.65 1.00 28.48 1.00 29.11 1.00 28.32 1.00 28.28
60	ATOM ATOM ATOM ATOM ATOM	9703 9704 9705 9706 9707	CD1 LEU CD2 LEU N HIS		66.102 65.650 64.906 69.178 70.073	64.833 1 65.377 1 64.302 1 66.229 1 67.026 1	.02.044 .00.720 .02.821 .02.397	1.00 28.91 1.00 26.67 1.00 27.26 1.00 29.12 1.00 28.26
65	ATOM ATOM ATOM	9708 9709 9710 9711	C HIS O HIS CB HIS CG HIS	B 483 B 483 B 483 B 483	69.396 68.454 71.131 72.123	68.181 1 68.801 1 67.637 1 66.657 1	.03.927 .03.416 .02.290 .01.762	1.00 28.26 1.00 28.91 1.00 27.89 1.00 28.44 1.00 27.09
70	ATOM ATOM ATOM ATOM ATOM	9712 9713 9714 9715 9716	ND1 HIS CD2 HIS CE1 HIS NE2 HIS	B 483 B 483 B 483	73.793	66.011 1 66.179 1 65.191 1 65.278 1	00.548 02.303 00.362 01.408	1.00 29.70 1.00 27.79 1.00 30.77 1.00 26.04
		2,10	N SER	B 484	69.944	68.538 1	U5.085	1.00 29.00

	ATOM	9717	CA	SER B		69.468	69.698		1.00 29.39
	ATOM	9718 9719	C O	SER B		70.397 71.614	70.903 70.785	105.664 105.718	1.00 29.47 1.00 27.76
	ATOM ATOM	9720	СВ	SER B		69.306	69.338	107.296	1.00 27.70
5	ATOM	9721	ŌĞ	SER B		69.382	70.500	108.077	1.00 32.58
	ATOM	9722	N	SER B		69.807	72.066	105.400	1.00 30.49
	ATOM ATOM	9723 9724	CA C	SER B		70.572 71.282	73.268 73.943	105.094 106.272	1.00 31.59 1.00 33.08
	ATOM	9725	Ö	SER B		72.350	74.536	106.096	1.00 33.60
10	ATOM	9726	ČВ	SER B		69.661	74.289	104.418	1.00 31.58
	ATOM	9727	OG	SER B		69.465	73.987	103.049	1.00 31.48
	ATOM ATOM	9728 9729	N CA	VAL B		70.729 71.284	73.850 74.659	107.462 108.534	1.00 34.59 1.00 36.93
	ATOM	9730	C	VAL B		72.762	74.420	108.654	1.00 36.73
15	MOTA	9731	0	VAL B	486	73.536	75.376	108.644	1.00 37.87
	MOTA	9732	CB	VAL B		70.646 70.631	74.455 75.824	109.933 110.673	1.00 38.37 1.00 40.52
	ATOM ATOM	9733 9734	CG1 CG2	VAL B		69.283	73.863	10.673	1.00 40.32
	ATOM	9735	N	ASN B		73.149	73.163	108.782	1.00 36.88
20	ATOM	9736	CA	ASN B		74.559	72.803	108.783	1.00 37.65
•	ATOM ATOM	9737 9738	C	ASN B		74.925 75.924	71.855 71.176	107.656 107.720	1.00 37.06 1.00 36.28
	ATOM	9739	CB	ASN B		74.953	72.198	110.124	1.00 38.31
	ATOM	9740	CG	ASN B	487	75.105	73.257	111.203	1.00 42.08
25	ATOM	9741		ASN B		74.366	73.264	112.190 111.002	1.00 45.04 1.00 44.16
	ATOM ATOM	9742 9743	ND2	ASN B ASP B		76.044 74.104	74.175 71.813	106.621	1.00 44.16
	ATOM	9744	CA	ASP B		74.351	70.945	105.488	1.00 36.95
	ATOM	9745	C	ASP B		74.672	69.537	105.924	1.00 36.35
30	ATOM	9746	0	ASP B		75.630 75.479	68.959 71.483	105.452 104.624	1.00 36.59 1.00 36.37
	ATOM ATOM	9747 9748	CB CG	ASP B		75.113	72.793	104.024	1.00 36.37
	ATOM	9749		ASP B	488	74.391	72.777	102.954	1.00 32.54
25	ATOM	9750	OD2	ASP B		75.479	73.886	104.423	1.00 34.83
35	ATOM ATOM	9751 9752	N CA	LYS B		73.878 74.103	68.995 67.639	106.828 107.249	1.00 35.78 1.00 36.75
	ATOM	9753	C	LYS B		73.393	66.684	106.292	1.00 35.41
	ATOM	9754	0	LYS B		72.326	67.022	105.761	1.00 33.88
40	ATOM ATOM	9755 9756	CB	LYS B		73.583 73.970	67.402 66.006	108.665 109.152	1.00 37.41 1.00 43.10
40	ATOM	9757	CG CD	LYS B		73.970	65.802	110.666	1.00 47.45
	ATOM	9758	CE	LYS B	489	74.643	64.498	111.029	1.00 49.75
	MOTA	9759	NZ	LYS B		73.966	63.784		1.00 52.01
45	ATOM ATOM	9760 9761	N CA	GLY B		74.010 73.389	65.519 64.429	106.069 105.323	1.00 33.74 1.00 33.26
13	ATOM	9762	C	GLY B		72.260	63.858	106.173	1.00 32.76
	MOTA	9763	0	GLY B		72.438		107.347	1.00 32.36
	ATOM ATOM	9764 9765	N CA	LEU B		71.055 69.974		105.636	1.00 33.01 1.00 33.73
50	ATOM	9766	C	LEU B		69.923		106.250	1.00 34.58
	MOTA	9767	0	LEU B		69.950	60.918	107.206	1.00 32.32
	MOTA	9768	CB	LEU B		68.624		106.026	1.00 33.78 1.00 36.24
	ATOM ATOM	9769 9770	CG CD1	LEU B		68.517 67.357		106.584 105.994	1.00 36.24
55	ATOM	9771	CD2	LEU B	491	68.376		108.117	1.00 38.67
	MOTA	9772	N	ARG B	492	69.904		104.982	1.00 35.31
	MOTA	9773	CA	ARG B		69.635 70.301		104.603 103.277	1.00 36.20 1.00 36.65
	ATOM ATOM	9774 9775	C O	ARG B		70.301	59.591 60.333	103.277	1.00 30.03
60	MOTA	9776	СВ	ARG B	492	68.153	59.765	104.305	1.00 36.71
	ATOM	9777	CG	ARG B		67.302		105.321	1.00 38.38
	ATOM	9778 9779	CD NE	ARG B		65.846 65.740		105.368 106.570	1.00 37.82 1.00 37.08
	ATOM ATOM	9780	CZ	ARG B	492	65.113		106.576	1.00 37.00
65	MOTA	9781	NH1	ARG B	492	64.458	62.231	105.651	1.00 37.47
	ATOM	9782		ARG B		65.141	62.343	107.836	1.00 37.23
	ATOM ATOM	9783 9784	N CA	VAL B	493 493	69.743 70.026		102.634 101.285	1.00 34.01 1.00 31.94
	ATOM	9785	C	VAL B		68.606		100.799	1.00 30.58
70	MOTA	9786	0	VAL B	493	67.872	57.111	101.479	1.00 29.50

	ATOM	9787			B 493	70.865		101.237	1.0	0 32.57
	ATOM ATOM	9788 9789			B 493	70.785				
	ATOM	9790			B 493 B 494	72.359 68.182				0 30.30 0 29.23
5		9791	CA	LEU	B 494	66.841		99.168		28.90
	ATOM	9792			B 494	66.799		98.178	1.00	28.74
	ATOM ATOM	9793 9794	_		B 494 B 494	65.873		98.206		
	ATOM	9795			B 494	66.238 66.174		98.529 99.513		
10		9796	CD1	LEU	B 494	66.005	61.778	98.767		
	ATOM	9797			B 494	65.057		100.491	1.00	28.40
	MOTA MOTA	9798 9799	N CA		B 495 B 495	67.786		97.302	1.00	28.15
	ATOM	9800	C		B 495	67.887 69.337		96.379 95.978		27.95 28.14
15		9801	0	GLU	B 495	69.961		95.595	1.00	
	ATOM ATOM	9802	CB		B 495	67.032	55.973	95.150	1.00	_
	ATOM	9803 9804	CG CD		B 495 B 495	67.354 66.934	55.054 53.629	93.983	1.00	
	ATOM	9805		GLU		65.762	53.446	94.279 94.588	1.00	
20	MOTA	9806	OE2		B 495	67.775	52.715	94.225	1.00	
	ATOM ATOM	9807 9808	N		B 496	69.892	54.384	96.073	1.00	
	ATOM	9809	CA C	ASP	B 496 B 496	71.311 71.593	54.212 53.254	95.778 94.667	1.00	29.15 29.08
	ATOM	9810	ŏ	ASP .	в 496	72.753	52.957	94.382		28.40
25	ATOM	9811	CB		B 496	72.096	53.812	97.023		29.89
•	ATOM ATOM	9812 9813	CG OD1	ASP :	B 496	71.724 71.067	52.460	97.552	1.00	
	ATOM	9814		ASP :		72.039	51.659 52.119	96.856 98.687		35.67 34.89
	ATOM	9815	N	ASN :	B 497	70.517	52.797	94.026		30.29
30	ATOM ATOM	9816	CA	ASN I		70.582	51.889	92.893	1.00	29.79
	ATOM	9817 9818	C O	ASN I		71.361 71.994	50.576 50.019	93.166 92.256		30.49
	ATOM	9819	ČВ	ASN I		71.171	52.639	91.702	1.00	30.08 30.35
2.5	ATOM	9820	CG	ASN I		70.102	53.332	90.851	1.00	30.90
35	ATOM ATOM	9821 9822		ASN I		69.234	52.671	90.257		32.35
	ATOM	9823	N ND2	SER I		70.201 71.332	54.647 50.098	90.732 94.415		30.45 31.45
	MOTA	9824	CA	SER F	3 498	71.999	48.843	94.787		32.80
40	ATOM ATOM	9825	C .	SER I		71.441	47.651	93.976	1.00	33.07
40	ATOM	9826 9827	O . CB	SER E		72.184 71.924	46.767 48.571	93.603 96.304		32.06
	ATOM	9828		SER E		70.582	48.684	96.811		33.14 35.98
	ATOM	9829		ALA E		70.158	47.673	93.627	1.00	33.72
45	ATOM ATOM	9830 9831		ALA E		69.624 70.327	46.581 46.512	92.847		34.12
	ATOM	9832		ALA E		70.775	45.437	91.515 91.109		34.76 34.90
	ATOM	9833		ALA E		68.133	46.713	92.645		34.02
	ATOM ATOM	9834 9835	~-	LEU E		70.457	47.660	90.848		35.42
50	ATOM	9836		LEU E		71.099 72.545	47.714 47.234	89.528 89.678		35.59 35.28
	MOTA	9837		LEU B		73.070	46.446	88.882		34.53
	ATOM	9838		LEU E		71.062	49.159	88.981	1.00	34.97
	ATOM ATOM	9839 9840		LEU B LEU B		71.027 71.798	49.422	87.471		37.81
55	ATOM	9841		LEU B		71.798	50.707 48.241	87.044 86.654		37.23 36.80
	ATOM	9842	N .	ASP B	501	73.167	47.709	90.734		35.54
	ATOM ATOM	9843 9844		ASP B		74.569	47.395	91.038	1.00	36.79
	ATOM	9845		ASP B ASP B		74.796 75.735	45.879 45.371	91.053		36.68
60	ATOM	9846		ASP B		74.939	48.008	90.410 92.403	1.00	34.68 37.28
	ATOM	9847	CG Z	ASP B	501	76.433	47.924	92.714		39.44
	ATOM ATOM	9848 9849		ASP B		77.265	48.026	91.803	1.00	39.64
	ATOM	9850		ASP B LYS B		76.866 73.898	47.768 45.171	93.877		47.25
65	ATOM	9851		LYS B		73.838	43.718	91.744 91.841		37.33 39.36
	ATOM	9852	C 1	LYS B	502	73.823	43.087	90.464		38.86
	ATOM ATOM	9853 9854		LYS B		74.649	42.281	90.098	1.00	37.72
	ATOM	9855		JYS B		73.046 73.774	43.111 43.104	92.925 94.326	1.00	39.93
70	ATOM	9856		LYS B		72.979	42.616	95.592	1.00	

	ATOM	9857	CE	LYS	в 502	73.659	43.132	96.928	1.00	52.43
	ATOM	9858	NZ	LYS	B 502	73.915	42.088	98.002	1.00	52.50
	MOTA	9859	N		B 503	72.807	43.489	89.699		38.71
	ATOM	9860	CA		B 503	72.674	42.995	88.322		39.36
5	ATOM	9861	C		B 503	73.907	43.319	87.458		38.16
	ATOM	9862	0		B 503	74.358	42.498	86.698		38.26
	ATOM	9863	CB		B 503	71.441	43.584	87.651		39.98
	ATOM ATOM	9864 9865	CG SD		B 503 B 503	70.136 68.772	42.959 43.508	88.096 87.082		44.31 51.44
10	ATOM	9866	CE		B 503	68.643	45.197	87.624		52.23
10	ATOM	9867	N		B 504	74.492	44.497	87.592		38.11
	ATOM	9868	CA		B 504	75.578	44.868	86.672		37.49
	ATOM	9869	C		B 504	76.902	44.113	86.877		38.02
	ATOM	9870	ō		B 504	77.662	43.874	85.915		36.62
15	ATOM	9871	СВ	LEU	B 504	75.778	46.381	86.679		36.89
	ATOM	9872	CG	LEU	B 504	74.661	47.111	85.894	1.00	36.85
	ATOM	9873		LEU		74.774	48.625	86.012		36.54
	MOTA	9874	CD2	LEU		74.606	46.721	84.398		36.84
	ATOM	9875	N		B 505	77.151	43.715	88.125		38.71
20	ATOM	9876	CA		B 505	78.328	42.934	88.458		39.81
	ATOM	9877	C		B 505	78.379	41.669	87.594		39.33
	ATOM ATOM	9878 9879	O CB		B 505 B 505	79.428 78.398	41.163 42.623	87.366 89.983		37.85 40.66
	ATOM	9880	CG		B 505	78.882	43.837	90.863		43.70
25	ATOM	9881	CD		B 505	78.675	43.624	92.373		48.71
	ATOM	9882	OE1		B 505	78.565	42.483	92.828		53.18
	ATOM	9883	NE2		B 505	78.609	44.725	93.148		50.14
	ATOM	9884	N		B 506	77.238	41.162	87.126	1.00	40.26
	ATOM	9885	CA	ASN	B 506	77.246	40.027	86.185	1.00	40.96
30	MOTA	9886	С		B 506	77.392	40.357	84.692		39.89
	ATOM	9887	0		B 506	77.086	39.526	83.856		41.00
	MOTA	9888	CB	ASN		75.991	39.186	86.344		41.01
	ATOM	9889	CG		B 506	75.866	38.596	87.737		44.86
35	ATOM	9890		ASN ASN		76.847 74.660	38.085	88.280 88.336		47.76
33	ATOM ATOM	9891 9892	N N		B 500	77.846	38.685 41.541	84.326		45.29 39.73
	ATOM	9893	CA	VAL		77.972	41.834	82.899		39.73
	ATOM	9894	C	VAL		79.276	42.499	82.603		38.86
	ATOM	9895	ŏ	VAL		79.876	43.126	83.464		38.82
40	ATOM	9896	CB	VAL	в 507	76.728	42.619	82.312	1.00	39.16
	MOTA	9897	CG1	VAL	B 507	76.185	43.507	83.274		39.25
	ATOM	9898	CG2	VAL		77.074	43.370	81.001		39.86
	ATOM	9899	N		B 508	79.764	42.299	81.397		38.32
45	MOTA	9900	CA		B 508	81.007	42.929	81.008		38.75
45	ATOM ATOM	9901 9902	C O		B 508 B 508	80.707 80.597	44.357 44.636	80.558 79.384		38.50 38.85
	ATOM	9903	СВ		B 508	81.712	42.146	79.364		38.76
	ATOM	9904	CG	GLN :		81.790	40.648	80.165		39.75
	ATOM	9905	CD		B 508	82.822	39.949	79.313		38.27
50	ATOM	9906		GLN		83.768	40.560	78.850		39.71
	MOTA	9907		GLN I		82.637	38.668	79.114		38.73
	ATOM	9908	N	MET :		80.585	45.246	81.527		38.00
	ATOM	9909	CA	MET :		80.310	46.635	81.267		37.57
	ATOM	9910	C	MET :		81.524	47.344	80.710		36.16
55	ATOM	9911	0_	MET I		82.628	47.031	81.051		36.25
	ATOM	9912	CB	MET I		79.876	47.311	82.560		37.43
	ATOM	9913	CG	MET I		78.539	46.824	83.006 81.754		38.53 42.19
	ATOM ATOM	9914 9915	SD CE	MET I		77.297 77.117	47.127 48.812	81.754		41.34
60	ATOM	9916	N	PRO I		81.300	48.300	79.831		34.57
00	ATOM	9917	CA	PRO I		82.376	49.102	79.288		33.86
	ATOM	9918	C	PRO		82.774	50.098	80.333		32.76
	ATOM	9919	ŏ	PRO		82.014	50.241	81.244		31.08
	MOTA	9920	CB	PRO I		81.700	49.901	78.187		33.77
65	ATOM	9921	CG	PRO 1		80.316	49.835	78.421	1.00	33.46
	MOTA	9922	CD	PRO I		79.990	48.710	79.336		34.56
	ATOM	9923	N	SER I		83.899	50.774	80.166		32.79
	ATOM	9924	CA	SER I		84.280	51.877	81.033		33.68
70	MOTA	9925	C	SER I		84.307	53.151	80.178		34.32
70	ATOM	9926	0	SER I	2 2TT	84.276	53.084	78.955	T.00	33.49

	ATOM	9927	СВ	SER B 511	85.686	5 51.678	81.567	1.00 33.29
	MOTA	9928		SER B 511				
	ATOM	9929		LYS B 512		54.284		
-	ATOM	9930		LYS B 512			80.247	
5		9931		LYS B 512				1.00 35.24
	ATOM ATOM	9932		LYS B 512				
	ATOM	9933 9934		LYS B 512			80.747	
	ATOM	9934	CG CD	LYS B 512	82.882			
10		9936	CE	LYS B 512 LYS B 512	81.520		80.523	1.00 31.54
	ATOM	9937	NZ	LYS B 512	81.212 79.844		79.895	1.00 31.66
	ATOM	9938	N	LYS B 513	86.308		80.379 79.588	1.00 30.48
	ATOM	9939	CA	LYS B 513	87.422		79.789	1.00 34.66 1.00 34.55
	ATOM	9940	C	LYS B 513	86.985		79.377	1.00 34.55 1.00 33.27
15	ATOM	9941	Ö	LYS B 513	86.400		78.302	1.00 33.27
	ATOM	9942	CB	LYS B 513	88.582		78.914	1.00 35.28
	MOTA	9943	CG	LYS B 513	89.911		79.360	1.00 38.42
	MOTA	9944	CD	LYS B 513	90.834		78.151	1.00 42.99
20	ATOM	9945	CE	LYS B 513	92.356		78.533	1.00 43.66
20	ATOM	9946	NZ	LYS B 513	93.216		77.286	1.00 45.03
	ATOM ATOM	9947	N	LEU B 514	87.317		80.225	1.00 31.88
	ATOM	9948 9949	CA	LEU B 514	87.053		80.103	1.00 32.15
	ATOM	9949	C	LEU B 514	88.411		80.196	1.00 32.80
25	ATOM	9951	O CB	LEU B 514 LEU B 514	89.101	62.203	81.224	1.00 31.05
	ATOM	9952	CG	LEU B 514	86.226	62.083	81.299	1.00 32.55
	ATOM	9953	CD1		85.150 84.978	63.166 63.884	81.171	1.00 35.94
	ATOM	9954	CD2		85.384	64.165	82.488 80.046	1.00 35.20 1.00 37.34
	ATOM	9955	N	ASP B 515	88.803	63.044	79.154	1.00 37.34 1.00 33.60
30	ATOM	9956	CA	ASP B 515	90.157	63.628	79.091	1.00 33.00
	ATOM	9957	C	ASP B 515	90.149	64.734	78.048	1.00 33.67
	ATOM	9958	0	ASP B 515	89.094	65.114	77.563	1.00 32.82
	MOTA	9959	CB	ASP B 515	91.142	62.547	78.675	1.00 34.54
25	ATOM	9960	CG	ASP B 515	92.569	62.806	79.134	1.00 37.60
35	ATOM	9961	OD1		92.889	63.930	79.590	1.00 37.94
	ATOM ATOM	9962	OD2		93.428	61.893	79.085	1.00 39.77
	ATOM	9963 9964	N CA	PHE B 516	91.307	65.257	77.690	1.00 34.11
	ATOM	9965	CA	PHE B 516 PHE B 516	91.348 92.548	66.335	76.720	1.00 35.27
40	ATOM	9966	ŏ	PHE B 516	93.502	66.256 65.580	75.791	1.00 36.20
	ATOM	9967	ČВ	PHE B 516	91.345	67.673	76.089 77.432	1.00 35.24 1.00 35.14
	ATOM	9968	CG	PHE B 516	92.512	67.863	78.341	1.00 35.14
	ATOM	9969	CD1	PHE B 516	93.738	68.247	77.843	1.00 37.49
	MOTA	9970	CD2	PHE B 516	92.400	67.606	79.709	1.00 37.60
45	ATOM	9971		PHE B 516	94.831	68.408	78.699	1.00 39.15
	ATOM	9972		PHE B 516	93.484	67.777	80.558	1.00 37.83
	ATOM	9973	CZ	PHE B 516	94.690	68.171	80.062	1.00 38.26
	ATOM ATOM	9974	N	ILE B 517	92.436	66.922	74.638	1.00 37.39
50	ATOM	9975 9976	CA	ILE B 517 ILE B 517	93.513	67.051	73.677	1.00 38.97
50	ATOM	9977	С 0	ILE B 517	93.673 92.835	68.531	73.511	1.00 39.81
	ATOM	9978	СВ	ILE B 517	93.203	69.307 66.452	73.953	1.00 39.05
	ATOM	9979		ILE B 517	91.788	66.798	72.271 71.825	1.00 39.15 1.00 39.44
	ATOM	9980		ILE B 517	93.393	64.974	72.266	1.00 39.44
55	ATOM	9981	CD1	ILE B 517	91.429	66.206	70.534	1.00 40.32
	ATOM	9982	N	ILE B 518	94.752	68.900	72.846	1.00 40.73
	ATOM	9983	CA	ILE B 518	95.088	70.276	72.615	1.00 41.90
	ATOM	9984	С	ILE B 518	94.874	70.476	71.158	1.00 42.73
	ATOM	9985	0	ILE B 518	95.324	69.688	70.362	1.00 44.34
60	ATOM	9986		ILE B 518	96.573	70.515	72.897	1.00 42.61
	ATOM	9987		ILE B 518	96.979	69.981	74.279	1.00 41.35
	ATOM	9988		ILE B 518	96.920	71.993	72.712	1.00 43.42
	ATOM	9989		ILE B 518	96.412	70.764	75.432	1.00 40.08
65	ATOM ATOM	9990		LEU B 519	94.162	71.503	70.788	1.00 43.62
03	ATOM	9991 9992		LEU B 519	94.045	71.842	69.387	1.00 44.63
	ATOM	9992 9993		LEU B 519	94.407	73.301	69.372	1.00 44.70
	ATOM	9994		LEU B 519 LEU B 519	93.726	74.111	69.973	1.00 43.61
	ATOM	9995		LEU B 519 LEU B 519	92.621 92.252	71.638 70.377	68.847	1.00 44.70
70	ATOM	9996		LEU B 519	92.594	69.095	68.061	1.00 46.16
		· =			22.334	55.055	68.773	1.00 47.42

	ATOM ATOM ATOM	9997 9998 9999	CD2 N CA	ASN ASN	B B	520 520	90.767 95.531 95.927	70.403 73.623 75.005	67.732 68.747 68.595	1.00 1.00	
5	ATOM ATOM ATOM ATOM	10000 10001 10002 10003	C O CB CG	ASN ASN	B B	520 520 520 520	95.971 95.267 94.967 95.511	75.772 76.770 75.712 75.757	69.875 70.030 67.629 66.248	1.00	46.05 46.58 46.98 49.34
10	ATOM ATOM ATOM	10004 10005 10006	OD1 ND2 N	ASN ASN GLU	B B	520 520 521	96.647 94.742 96.781	75.308 76.314 75.311	66.033 65.291 70.803	1.00 1.00 1.00	51.14 49.12 45.72
	ATOM ATOM ATOM ATOM	10007 10008 10009 10010	CA C O CB	GLU GLU	B B	521 521	96.954 95.832 95.960 97.053	76.038 75.864 76.346 77.555	72.054 73.051 74.189 71.797	1.00 1.00	45.79 44.04 45.10 47.02
15	ATOM ATOM ATOM ATOM	10011 10012 10013 10014	CG CD OE1 OE2		B B	521 521	98.446 98.397 97.369 99.397	78.176 79.707 80.234 80.385	71.813 71.986 72.479 71.635	1.00	50.35 53.77 51.60 57.13
20	ATOM ATOM ATOM	10015 10016 10017	N CA C	THR THR THR	B B B	522 522 522	94.716 93.586 93.209	75.247 75.164 73.746	72.661 73.595 74.005	1.00 1.00 1.00	41.38 38.96 36.68
25	ATOM ATOM ATOM	10018 10019 10020 10021	O CB OG1 CG2		B B	522 522	93.399 92.328 92.560 91.126	72.791 75.864 77.277 75.759	73.270 72.997 72.831 73.977	1.00 1.00	34.63 39.60 38.31 38.25
23	ATOM ATOM ATOM	10022 10023 10024	N CA C	LYS LYS LYS	B B B	523 523 523	92.637 92.145 90.781	73.634 72.359 72.060	75.192 75.667 75.086	1.00 1.00 1.00	34.80 33.28 30.81
30	ATOM ATOM ATOM	10025 10026 10027 10028	O CB CG CD	LYS LYS LYS	B B	523 523	89.830 91.939 93.135 92.604	72.859 72.389 72.259 72.123	75.224 77.167 78.039 79.487	1.00 1.00	28.33 33.48 37.54 41.59
35	ATOM ATOM ATOM	10029 10030 10031	CE NZ N	LYS LYS PHE	B B	523 523	93.644 92.930 90.641	71.666 71.329 70.889	80.482 81.773 74.494	1.00 1.00	45.90 48.02 29.69
	ATOM ATOM ATOM	10032 10033 10034	CA C O	PHE PHE PHE	B B	524 524	89.278 89.023 89.818	70.448 69.054 68.140	74.102 74.626 74.403	1.00 1.00	29.81 28.20 28.48
40	ATOM ATOM ATOM	10035 10036 10037 10038	CB CG CD1 CD2	PHE PHE PHE PHE	B B	524 524 524 524	89.100 89.034 87.851 90.146	70.495 71.877 72.583 72.466	72.623 72.082 72.101 71.536	1.00 1.00	29.61 31.07 30.34 30.96
45	ATOM ATOM ATOM	10039 10040 10041	CE1 CE2 CZ	PHE PHE	B B	524 524	87.806 90.087 88.933	73.832 73.723 74.402	71.632 71.051 71.079	1.00	30.24 29.57 28.05
	ATOM ATOM ATOM	10042 10043 10044 10045	N CA C O	TRP TRP TRP	B B	525 525	87.923 87.602 86.908 86.174	68.905 67.652 66.623 66.974	75.345 76.004 75.126 74.195	1.00	26.62 25.72 25.25 24.05
50	ATOM ATOM ATOM	10046 10047 10048	CB CG CD1	TRP TRP TRP	B B B	525 525 525	86.732 87.455 87.758	67.965 68.732 70.073	77.216 78.277 78.275	1.00 1.00 1.00	25.79 27.63 27.16
55	ATOM ATOM ATOM ATOM	10049 10050 10051 10052	CD2 NE1 CE2 CE3	TRP TRP TRP	B B	525 525	88.017 88.463 88.634 88.075	68.192 70.390 69.255 66.904	79.477 79.407 80.166 80.030	1.00 1.00	29.89 31.50 30.31 30.50
	ATOM ATOM ATOM	10053 10054 10055	CZ2 CZ3 CH2	TRP TRP TRP	B B B	525 525 525	89.270 88.697 89.290	69.086 66.730 67.823	81.386 81.249 81.923	1.00 1.00	30.73 31.25 31.94
60	ATOM ATOM ATOM	10056 10057 10058 10059	N CA C O	TYR TYR TYR TYR	B B	526 526	87.121 86.422 86.160 86.720	65.356 64.269 63.161 63.184	75.449 74.801 75.804 76.895	1.00 1.00	24.69 25.76 25.33 25.36
65	ATOM ATOM ATOM	10060 10061 10062	CB CG CD1	TYR TYR	B B	526 526	87.260 88.489 89.675	63.675 62.959 63.649	73.664 74.141 74.354	1.00 1.00	26.43 29.07 30.32
70	ATOM ATOM ATOM ATOM	10063 10064 10065 10066	CD2 CE1 CE2 CZ	TYR TYR TYR TYR	B B	526 526	88.466 90.807 89.594 90.772	61.605 63.009 60.943 61.657	74.380 74.809 74.818 75.029	1.00 1.00	32.46 32.27 36.27 36.33
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5	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1 10068 1 10069 1 10070 1 10071 1 10072	N CA C C CB	TYR B 52 GLN B 52 GLN B 52 GLN B 52 GLN B 52 GLN B 52 GLN B 52	7 7 7 1	91.899 85.284 85.060 85.163 84.866 83.670	62.222 60.994 59.824 59.952 60.932	75.439 76.189 75.238 74.021 76.904	1.00 25.09 1.00 25.08 1.00 26.26 1.00 26.67 1.00 25.67
10	ATOM ATOM	10074 10075 10076 10077 10078	CD OE1 NE2 N CA	GLN B 527 GLN B 527 GLN B 527 MET B 528 MET B 528	7 7 1	82.391 81.106 80.956 80.187 85.608 85.525	60.932 61.540 60.047 58.691 57.424	76.867 77.952 76.379 75.773 75.062	1.00 26.97 1.00 24.92 1.00 24.49 1.00 27.54 1.00 28.64
15	ATOM ATOM ATOM ATOM ATOM	10080 10081 10082 10083	C O CB CG SD	MET B 528		84.841 85.150 86.891 87.784 89.285	56.371 56.202 56.882 57.848 57.067	75.930 77.127 74.673 73.914 73.244	1.00 28.90 1.00 28.28 1.00 28.81 1.00 31.74 1.00 29.83
20	ATOM ATOM ATOM ATOM ATOM		CE N CA C	MET B 528 ILE B 529 ILE B 529 ILE B 529 ILE B 529		89.692 83.915 83.330 84.141 84.114	58.217 55.659 54.488 53.290 52.986	72.070 75.312 75.899 75.398 74.198	1.00 29.90 1.00 29.12 1.00 29.94 1.00 30.98 1.00 30.01
25	ATOM ATOM ATOM ATOM ATOM	10099 10091 10092 10093 10094	CB CG1 CG2 CD1 N	ILE B 529 ILE B 529 LEU B 530		81.866 81.154 81.281 79.855 84.865	54.401 55.633 53.175 55.866 52.626	75.481 76.046 76.084 75.526 76.311	1.00 30.15 1.00 32.73 1.00 29.20 1.00 37.12 1.00 31.29
30	ATOM ATOM ATOM ATOM	10095 10096 10097 10098	CA C O CB CG	LEU B 530 LEU B 530 LEU B 530 LEU B 530 LEU B 530		85.788 85.256 84.612 87.140 87.690	51.554 50.178 49.949 51.727 53.151	75.924 76.240 77.283 76.613 76.564	1.00 31.73 1.00 31.76 1.00 32.88 1.00 32.22 1.00 33.27
35	ATOM ATOM ATOM ATOM ATOM	10099 10100 10101 10102 10103	CD2 N CA C	LEU B 530 LEU B 530 PRO B 531 PRO B 531 PRO B 531		88.595 88.414 85.511 85.110 85.674	53.449 53.337 49.245 47.863 47.323	77.722 75.272 75.346 75.585 76.913	1.00 35.58 1.00 34.59 1.00 31.94 1.00 32.83 1.00 33.43
40	ATOM ATOM ATOM ATOM ATOM	10104 10105 10106 10107 10108	O CB CG CD N	PRO B 531 PRO B 531 PRO B 531 PRO B 531 PRO B 532		86.714 85.738 85.898 86.176 85.012	47.735 47.102 48.097 49.419 46.330	77.390 74.417 73.360 74.045 77.443	1.00 31.92 1.00 32.20 1.00 32.54 1.00 32.48 1.00 35.12
45	ATOM ATOM ATOM ATOM ATOM	10109 10110 10111 10112 10113	CA C O CB CG	PRO B 532 PRO B 532 PRO B 532 PRO B 532 PRO B 532		85.471 86.816 87.105 84.402 83.577	45.710 45.052 44.764 44.675 44.523	78.677 78.373 77.204 78.985 77.738	1.00 37.14 1.00 38.82 1.00 39.18 1.00 37.36
50	ATOM ATOM ATOM ATOM ATOM	10114 10115 10116 10117 10118	CD N CA C	PRO B 532 HIS B 533 HIS B 533 HIS B 533 HIS B 533		83.878 87.640 88.966 89.682 90.328	45.636 44.862 44.280 45.018 44.421	76.816 79.396 79.212 78.103 77.263	1.00 36.74 1.00 35.14 1.00 41.03 1.00 42.46 1.00 43.42 1.00 44.13
55	ATOM ATOM ATOM ATOM ATOM	10119 10120 10121 10122 10123	CB CG ND1 CD2	HIS B 533 HIS B 533 HIS B 533 HIS B 533 HIS B 533		88.854 88.023 87.031 88.016 86.454	42.805 42.033 41.164 42.023 40.639	78.863 79.831 79.437 81.184 80.505	1.00 44.13 1.00 42.84 1.00 43.24 1.00 43.68 1.00 46.76 1.00 44.62
60	ATOM ATOM ATOM ATOM ATOM	10124 10125 10126 10127 10128	NE2 N CA C	HIS B 533 PHE B 534 PHE B 534 PHE B 534 PHE B 534		87.028 89.531 90.203 91.678 92.276	41.150 46.326 47.128 46.784	81.578 78.083 77.080 77.047	1.00 46.14 1.00 43.97 1.00 44.87 1.00 45.83
65	ATOM ATOM ATOM ATOM ATOM	10129 10130 10131 10132 10133	CB CG CD1 CD2	PHE B 534 PHE B 534 PHE B 534 PHE B 534 PHE B 534		90.040 90.647 90.300 91.558 90.844	46.550 48.594 49.507 49.438 50.466 50.306	78.082 77.432 76.454 75.124 76.863 74.200	1.00 46.41 1.00 44.17 1.00 44.16 1.00 45.18 1.00 45.36 1.00 45.22
70	ATOM ATOM ATOM	10134 10135 10136	CE2	PHE B 534 PHE B 534 ASP B 535		92.107 91.745 92.281	51.337 51.248 46.770	75.958 74.602 75.871	1.00 46.95 1.00 46.30 1.00 46.97

	ATOM ATOM	10137 10138	CA C	ASP ASP	B B	535 535	93.705 94.317	46.471 47.342	75.775 74.721	1.00	47.32 47.18
	ATOM	10139	ŏ		В	535	94.052	47.138	73.557	1.00	46.48
	ATOM	10140	CB	ASP	В	535	93.932	45.013	75.400	1.00	
5	ATOM	10141	CG		В	535	95.405	44.720	75.057		49.55
	ATOM	10142		ASP		535	96.253	45.647	75.162		50.88
	ATOM	10143	_	ASP		535	95.797	43.608 48.297	74.653		49.67
	ATOM	10144 10145	N CA	LYS LYS		536 536	95.150 95.718	48.297	75.126 74.195		47.86 48.50
10	ATOM ATOM	10145	CA	LYS		536	96.760	48.780	73.184		48.52
10	ATOM	10147	ŏ	LYS		536	97.236	49.576	72.363		47.71
	ATOM	10148	ČВ		В	536	96.286	50.480	74.944		49.03
	ATOM	10149	CG	LYS		536	97.480	50.191	75.880	1.00	52.28
	ATOM	10150	CD	LYS	В	536	97.644	51.365	76.881		55.15
15	MOTA	10151	CE	LYS		536	98.639	51.039	78.025		57.36
	ATOM	10152	NZ	LYS		536	98.718	52.151	79.040	1.00	56.81
	MOTA	10153	N	SER		537 537	97.103	47.496 46.973	73.210 72.208	$1.00 \\ 1.00$	48.46 49.13
	ATOM ATOM	10154 10155	CA C	SER SER		537	98.028 97.243	46.475	70.993		49.13
20	ATOM	10156	Ö	SER		537	97.824	45.991	70.009		49.23
20	ATOM	10157	ČВ	SER		537	98.896	45.860	72.785		49.28
	ATOM	10158	OG	SER		537	98.097	44.746	73.152		50.50
	ATOM	10159	N	LYS	В	538	95.916	46.590	71.063		48.47
	MOTA	10160	CA	LYS		538	95.075	46.210	69.931		47.89
25	MOTA	10161	C	LYS		538	94.537	47.443	69.249		46.38
	ATOM	10162	0	LYS		538	94.581	48.545	69.788		46.40
	ATOM	10163 10164	CB CG	LYS LYS		538 538	93.899 94.264	45.336 43.869	70.373 70.583	1.00	
	ATOM ATOM	10165	CD	LYS		538	93.423	43.238	71.688		52.37
30	ATOM	10166	CE	LYS		538	94.133	42.062	72.398		53.34
	ATOM	10167	NZ	LYS		538	93.285	40.818	72.399		53.62
	ATOM	10168	N	LYS	В	539	94.022	47.262	68.050	1.00	44.87
	MOTA	10169	CA	LYS		539	93.405	48.369	67.358		43.55
	ATOM	10170	С	LYS		539	91.914	48.090	67.297		40.89
35	ATOM	10171	0	LYS		539	91.524	47.076	66.789		40.49
	ATOM	10172	CB	LYS		539	94.033	48.530	65.973 66.038	1.00	44.47 45.62
	ATOM ATOM	10173 10174	CG CD	LYS :		539 539	95.538 96.074	48.675 49.677	65.051		47.78
	ATOM	10174	CE			539	97.484	50.141	65.445		48.95
40	ATOM	10176	NZ	LYS			97.610	51.616	65.209		50.32
	ATOM	10177	N	TYR	В	540	91.100	48.969	67.889	1.00	38.45
	MOTA	10178	CA	TYR :		540	89.641	48.855	67.858	1.00	
	ATOM	10179	C	TYR :		540	89.085	49.795	66.805	1.00	
45	ATOM	10180	0	TYR :			89.690	50.825	66.525		33.35
45	ATOM ATOM	10181 10182	CB CG	TYR :		540	89.030 89.520	49.243 48.404	69.212 70.374		34.98 32.83
	ATOM	10182	CD1				90.776	48.578	70.885		33.15
	ATOM	10184		TYR			88.742		70.902		32.68
	ATOM	10185		TYR			91.228	47.809	71.912		34.42
50	ATOM	10186	CE2	TYR I			89.169	46.640	71.916		33.22
	ATOM	10187	CZ	TYR I			90.420	46.832	72.421		33.72
	ATOM	10188	ОН	TYR I			90.856	46.047	73.430		32.51
	MOTA	10189	N	PRO I			87.954 87.208	49.430	66.204		32.50 31.98
55	ATOM ATOM	10190 10191	CA C	PRO I			86.599	50.343 51.474	65.337 66.176		31.61
33	ATOM	10191	Ö	PRO I			86.225	51.267	67.314		31.17
	ATOM	10193	ČВ	PRO			86.109	49.453	64.786		32.02
	ATOM	10194	CG	PRO 1			85.926	48.454	65.866	1.00	32.49
	MOTA	10195	CD	PRO 1			87.305	48.111	66.277		32.29
60	MOTA	10196	N	LEU 1			86.537	52.671	65.619		31.70
	MOTA	10197	CA	LEU			86.027	53.796	66.352		31.15
	ATOM	10198	C	LEU I			84.801	54.432	65.736		30.44
	ATOM	10199	0	LEU 3			84.798	54.793	64.525		29.93 32.05
65	ATOM ATOM	10200 10201	CB CG	LEU I			87.102 86.691	54.872 55.940	66.465 67.489		34.95
03	ATOM	10201		LEU I			87.860	56.396	68.295		35.53
	ATOM	10203		LEU			86.030	57.086	66.798		35.86
	MOTA	10204	N	LEU	3	543	83.784	54.608	66.586		29.46
	MOTA	10205	CA	LEU I	3	543	82.586	55.368	66.227		29.14
70	MOTA	10206	С	LEU I	3	543	82.555	56.698	66.958	1.00	28.16

	ATOM	1 10207	0	LEU B 543	82.537	7 56.755	68.212	1 00 20 24
	ATOM		_					
			_		81.329			
	ATOM				80.002			1.00 30.86
_	ATOM		CD	1 LEU B 543	78.876	54.568	66.950	1.00 29.26
5	ATOM	10211	CD	2 LEU B 543	80.047			
	ATOM	10212	N	LEU B 544	82.536			
	ATOM	_						
	_				82.401		66.760	
	ATOM		-	LEU B 544	80.904		66.795	1.00 27.16
	ATOM		_	LEU B 544	80.256	59.720	65.735	1.00 26.33
10	ATOM	10216	CB	LEU B 544	83.171		65.918	1.00 26.04
	ATOM		CG	LEU B 544	83.254			
	ATOM						66.311	
				1 LEU B 544	84.240		67.414	1.00 28.08
	ATOM		CD:	2 LEU B 544	83.663	62.290	65.115	
	ATOM	10220	N	ASP B 545	80.377		68.019	
15	ATOM	10221	CA	ASP B 545	79.019			
	ATOM						68.320	1.00 26.49
			C	ASP B 545	79.052		68.519	1.00 26.44
	ATOM		О	ASP B 545	79.704	61.954	69.427	1.00 24.96
	ATOM	10224	CB	ASP B 545	78.543	59.222	69.552	1.00 26.52
	ATOM	10225	CG	ASP B 545	77.240		70.081	1 00 20.52
20	ATOM	10226		ASP B 545				1.00 28.25
20					76.638		69.494	1.00 31.33
	ATOM	10227	OD2		76.751		71.091	1.00 29.13
	ATOM	10228	N	VAL B 546	78.403	62.200	67.611	1.00 26.32
	ATOM	10229	CA	VAL B 546	78.468		67.571	1.00 26.13
	ATOM	10230	C	VAL B 546	77.144			
25	ATOM						67.756	1.00 25.53
23		10231	0	VAL B 546	76.100		67.300	1.00 25.95
	ATOM	10232	CB	VAL B 546	79.046	64.135	66.206	1.00 26.98
	ATOM	10233	CG1	. VAL B 546	78.388	63.436	65.031	1.00 29.08
	ATOM	10234	CG2		78.880			
	ATOM					65.635	66.016	1.00 27.58
20		10235	N	TYR B 547	77.173	65.525	68.423	1.00 25.15
30	ATOM	10236	CA	TYR B 547	76.002	66.388	68.456	1.00 25.44
	ATOM	10237	С	TYR B 547	76.560	67.668	67.953	1.00 25.50
	ATOM	10238	0	TYR B 547	76.371	67.991	66.794	
	ATOM	10239	ČВ	TYR B 547				1.00 24.39
					75.324	66.549	69.854	1.00 25.83
	ATOM	10240	CG	TYR B 547	74.125	67.470	69.728	1.00 26.34
35	ATOM	10241	CD1	TYR B 547	72.982	67.064	68.992	1.00 26.01
	ATOM	10242	CD2	TYR B 547	74.141	68.760	70.256	1.00 26.81
	ATOM	10243	CE1					
	ATOM				71.875	67.901	68.834	1.00 23.53
		10244	CE2		73.047	69.620	70.111	1.00 23.51
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45	ATOM	10251	CB	ALA B 548	79.087	69.238	67.493	1.00. 26.28
	ATOM	10252	N	GLY B 549	76.050	70.966		
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	ATOM	10260	CB	PRO B 550	75.212	76.869	69.264	1.00 28.88
55	ATOM	10261	CG	PRO B 550	74.711	76.461		
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	ATOM	10263	N	CYS B 551	76.579	75.576	72.190	1.00 28.41
	ATOM	10264	CA	CYS B 551	76.368	75.469	73.645	1.00 29.87
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	ATOM	10272	0	SER B 552	78.649	71.647	74.221	1.00 28.06
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V.

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	ATOM	10420	OG1			570	77.042	43.148	73.698		31.14
5	ATOM	10421	CG2			570	77.408	41.967	71.676		32.40
	ATOM	10422	N			571	80.065 80.789	44.565	70.725		32.39
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	ATOM	10424	Ö	GLU			82.988	45.068	68.655		33.65
10	ATOM	10426	СВ			571	80.072	45.657	68.587		32.41
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	ATOM	10428	CD			571	78.410	43.831	67.946		36.63
	ATOM	10429	OE1			571	79.270	43.253	67.270		39.21
	ATOM	10430		GLU			77.352	43.268	68.263		39.45
15	ATOM	10431	N			572	82.691	45.465	70.806		31.26 31.13
	ATOM ATOM	10432 10433	CA C			572 572	84.079 84.403	45.874 47.096	70.969 70.105		29.57
	ATOM	10433	0			572	85.478	47.208	69.542		29.37
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20	ATOM	10436	CG	ASN		572	84.926	43.593	71.821		32.45
	ATOM	10437	OD1	ASN	В	572	85.101	43.855	72.988	1.00	36.78
	ATOM	10438	ND2			572	84.548	42.384	71.420		33.77
	ATOM	10439	N			573	83.475	48.029	70.061		28.95
25	ATOM	10440	CA		-	573 573	83.682	49.287 50.419	69.383 70.382		29.13 28.98
25	ATOM ATOM	10441 10442	C O	ILE	_	573	83.934 83.268	50.419	70.362		28.09
	ATOM	10442	СВ	ILE		573	82.455	49.633	68.576		29.67
	ATOM	10444	CG1	ILE		573	82.180	48.531	67.555		30.91
	ATOM	10445	CG2	ILE	В	573	82.679	50.955	67.858		30.51
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	ATOM	10448	CA	ILE		574	85.116	52.446 53.511	70.856 70.370		28.11 27.24
	ATOM ATOM	10449 10450	C	ILE		574 574	84.162 84.158	53.815	69.187		27.24
35	ATOM	10451	СВ	ILE		574	86.569	52.940	70.662		28.66
	ATOM	10452	CG1	ILE		574	87.547	52.084	71.454		29.17
	ATOM	10453	CG2	ILE		574	86.740	54.365	71.206	1.00	30.07
	ATOM	10454	CD1	ILE		574	88.994	52.424	71.168		29.40
40	ATOM	10455	N	VAL		575	83.404	54.118	71.276		26.67
40	ATOM	10456	CA	VAL		575 575	82.464 82.890	55.191 56.485	70.921 71.557		26.59 25.86
	ATOM ATOM	10457 10458	C O	VAL VAL		575	82.791	56.645	72.765		26.51
	ATOM	10459	СВ	VAL		575	81.030		71.378		26.48
	ATOM	10460		VAL		575	80.097	56.070	70.967		27.49
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55	ATOM	10471	CB	SER			81.194	62.194	72.457		24.10
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60	ATOM	10476	ō	PHE			82.664	66.941	70.584		25.63
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                                                                         1.00 32.65
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ATOM 10558 CB. LYS B 589 88.72.64 82.380 73.678 1.00 34.26 ATOM 10560 CD. LYS B 589 88.765 82.367 73.573 1.00 37.2678 ATOM 10561 CB. LYS B 589 90.868 82.313 72.573 1.00 37.2731 ATOM 10562 NZ LYS B 589 90.868 82.367 73.123 1.00 42.91 ATOM 10562 NZ LYS B 589 90.868 82.367 73.123 1.00 42.91 ATOM 10563 N LIE B 590 85.255 79.980 73.105 1.00 43.08 ATOM 10566 CA. LIE B 590 85.255 79.980 73.105 1.00 43.08 ATOM 10566 CA. LIE B 590 85.050 77.705 1.00 30.127 ATOM 10566 CA. LIE B 590 85.050 77.705 1.00 30.127 ATOM 10566 CA. LIE B 590 85.025 77.594 1.00 30.127 ATOM 10567 CB. LIE B 590 85.322 77.594 1.00 30.127 ATOM 10568 CG. LIE B 590 85.322 77.594 1.00 30.61 ATOM 10567 CD. LIE B 590 85.322 77.594 1.00 30.61 ATOM 10567 CD. LIE B 590 86.870 77.484 73.670 1.00 28.65 ATOM 10570 CD. LIE B 590 87.277 76.467 73.078 1.00 26.65 ATOM 10571 N MET B 591 82.651 79.022 72.871 1.00 30.17 ATOM 10573 C MET B 591 82.651 79.022 72.871 1.00 30.17 ATOM 10573 C MET B 591 80.884 79.781 71.303 1.00 29.25 ATOM 10576 CB. MET B 591 80.884 79.781 71.303 1.00 29.25 ATOM 10576 CB. MET B 591 80.884 79.781 71.303 1.00 29.25 ATOM 10577 C MET B 591 80.884 79.781 71.303 1.00 29.25 ATOM 10578 CB. MET B 591 80.884 79.781 71.303 1.00 29.25 ATOM 10579 N MET B 591 80.884 79.781 71.303 1.00 29.25 ATOM 10579 N MET B 591 80.884 79.781 71.303 1.00 29.25 ATOM 10579 C MET B 591 77.284 80.660 74.802 1.00 29.62 ATOM 10587 C MET B 591 77.284 80.660 74.802 1.00 29.62 ATOM 10587 C MET B 591 77.284 80.660 74.802 1.00 29.62 ATOM 10589 C M HIS B 592 81.648 82.537 79.996 71.00 28.43 ATOM 10589 C M HIS B 592 81.648 82.537 79.996 71.00 28.43 ATOM 10589 C M HIS B 592 81.648 82.537 79.996 71.00 28.43 ATOM 10589 C M HIS B 592 81.648 82.537 79.996 71.00 28.43 ATOM 10589 C M HIS B 592 81.688 81.993 72.497 70.363 1.00 29.762 ATOM 10580 C M HIS B 592 81.688 80.686 6.509 1.00 27.76 ATOM 10580 C M HIS B 592 81.688 80.686 6.509 1.00 27.76 ATOM 10580 C M HIS B 592 81.688 80.686 6.509 1.00 27.76 ATOM 10580 C M HIS B 592 81.889 80.680 77.996 1.00 27.77 ATOM 10580 C M HIS B 594 81.889 80.680										
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ATOM								83.789	71.569	1.00 28.43
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ATOM 10617 NE ARG B 596 76.324 88.059 61.201 1.00 44.20 ATOM 10618 CZ ARG B 596 76.860 88.114 59.978 1.00 46.01 ATOM 10619 NH1 ARG B 596 78.084 87.620 59.739 1.00 47.70 ATOM 10620 NH2 ARG B 596 76.170 88.672 58.989 1.00 43.53 ATOM 10621 N ARG B 597 78.256 81.368 61.943 1.00 32.93 ATOM 10622 CA ARG B 597 79.043 80.476 61.081 1.00 34.19 ATOM 10623 C ARG B 597 78.829 78.990 61.332 1.00 32.69 ATOM 10624 O ARG B 597 79.796 78.272 61.458 1.00 32.70 ATOM 10625 CB ARG B 597 80.549 80.815 61.232 1.00 36.10	۲0									
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ATOM 10625 CB ARG B 597 80.549 80.815 61.232 1.00 36.10										
		ATOM								
	70	ATOM	10626	CG	ARG	в 597	80.956	82.200	60.699	1.00 41.65

:	MOTA MOTA MOTA MOTA MOTA MOTA MOTA	1 10628 1 10629 1 10630 1 10631 1 10632	NE CZ NHI NH2	ARG ARG L ARG P ARG LEU	B 597 B 597 B 597 B 597 B 597 B 598 B 598	82.277 82.324 82.566 82.767 82.613 77.575	82.880 84.023 85.173 84.014 78.525	62.755 63.421 62.766 64.750 61.381	1.00 1.00 1.00 1.00	63.35
10	ATOM ATOM ATOM ATOM	1 10634 1 10635 1 10636 1 10637 1 10638	C O CB CG CD1	LEU LEU LEU LEU	B 598 B 598 B 598 B 598 B 598	77.799 77.947 75.768 75.164 73.698	76.267 76.718 76.869 77.669 77.411		1.00 1.00 1.00	30.47
15	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	10640 10641 10642 10643	N CA C O	GLY GLY GLY	B 598 B 599 B 599 B 599 B 599	75.858 78.101 78.646 80.079 80.514	75.015 74.140 74.472 74.163	64.254 60.848 59.832 59.434 58.348	1.00 1.00 1.00 1.00	28.42 30.02 29.74 29.84 29.03
20	ATOM	10645 10646 10647		THR		80.844 82.196 83.197 83.554 82.100	75.444	60.348 60.022 61.038 60.949	1.00 1.00 1.00	30.03 29.73 29.64
25	ATOM ATOM	10649 10650 10651		THR THR PHE PHE		82.558 82.794 83.606 84.644 84.194	77.447 77.710 75.627 75.146	59.909 58.634 60.930 62.044 62.961 63.736	1.00 1.00	34.89 28.28 29.95 30.35
30	ATOM ATOM	10654 10655 10656 10657 10658	O CB CG	PHE PHE PHE	B 601 B 601 B 601	84.991 85.083 85.644 86.546 85.292	73.038 76.239 77.480 77.401	63.982 63.944 63.290 62.245	1.00 1.00 1.00	30.77 34.23 38.59
· 35	ATOM ATOM ATOM ATOM ATOM	10659 10660 10661 10662 10663	CE1 CE2 CZ N	PHE : PHE : PHE : GLU :	B 601 B 601 B 601 B 602	87.070 85.821 86.700 82.906	78.735 78.560 79.893 79.800 73.835	63.746 61.663 63.162 62.132 64.086	1.00 1.00 1.00 1.00	38.13 38.92 38.48 38.17 29.35
40	ATOM ATOM ATOM ATOM	10664 10665 10666 10667	CA C O CB CG	GLU I GLU I GLU I	B 602 B 602	82.423 82.525 82.773 81.000 79.859	72.673 71.384 70.290 72.916 72.581	64.819 63.979 64.510 65.356 64.437	1.00 1.00 1.00 1.00	28.58 28.39 28.66 28.78 27.88
45	ATOM ATOM ATOM ATOM ATOM ATOM	10668 10669 10670 10671 10672 10673	CD OE1 OE2 N CA C	GLU I GLU I GLU I VAL I VAL I	602 602 603 603	79.514 80.433 78.311 82.423 82.535 84.012	73.699 74.414 73.818 71.528 70.393 70.018	63.503 63.025 63.212 62.663 61.736 61.601	1.00 1.00 1.00 1.00	28.39 28.79 29.14 28.03 27.82 28.52
50	ATOM ATOM ATOM	10674 10675 10676 10677	CG2	VAL E VAL E VAL E	603 603 603	84.410 81.969 82.140 80.530	68.848 70.803 69.735 71.170	61.662 60.340 59.338 60.453	1.00 1.00 1.00	27.76 27.10 27.69 28.49
55	ATOM ATOM ATOM ATOM ATOM ATOM	10678 10679 10680 10681 10682 10683	CA C O CB	GLU E GLU E GLU E GLU E GLU E	604 604 604 604	84.818 86.261 86.855 87.694 86.895 86.525	71.036 70.877 70.214 69.330 72.253 72.986	61.361 61.261 62.486 62.376 61.125 59.830	1.00 1.00 1.00 1.00	29.64 30.17 29.17 26.66 31.80 35.77
60	ATOM ATOM ATOM ATOM ATOM	10684 10685 10686 10687 10688	OE1 OE2 N	GLU E GLU E GLU E ASP E	604 604 605	87.043 88.206 86.277 86.378	74.421 74.647 75.314 70.625	59.795 60.303 59.270 63.661	1.00 1.00 1.00 1.00	42.21 42.15 43.50 28.35
65	ATOM ATOM ATOM ATOM ATOM	10688 10690 10691 10692 10693	C O CB CG	ASP B ASP B ASP B ASP B ASP B	605 605 605 605	86.962 86.642 87.458 86.496 87.165 87.929	70.164 68.688 67.954 71.020 72.419 72.797	64.900 65.133 65.662 66.084 66.138 65.213	1.00 1.00 1.00	27.49 29.20 31.44
70	ATOM ATOM ATOM	10694 10695 10696	OD2	ASP B GLN B GLN B	605 606	86.931 85.462 85.127	73.228 68.242 66.838	67.085 64.730 64.861	1.00 1.00 1.00	30.59 27.69

	ATOM ATOM	10697 10698	C O	GLN E		86.104 86.541	66.041 64.963	63.985 64.357	1.00	27.77 27.24
	ATOM	10699	CB	GLN E	606	83.670	66.574	64.448	1.00	26.75
-	ATOM	10700	CG	GLN E		82.590	67.157	65.402	1.00	25.51 25.37
5	MOTA ATOM	10701 10702	CD OE1	GLN E		82.546 82.500	66.412 65.177	66.737 66.759		31.48
	ATOM	10702	NE2	GLN E		82.634	67.141	67.833	1.00	22.23
	ATOM	10704	N	ILE B		86.438	66.573	62.819	1.00	
	MOTA	10705	CA	ILE B		87.398	65.911	61.918	1.00	30.05
10	ATOM	10706	C	ILE B		88.787	65.823	62.484	1.00	30.76
	ATOM	10707 10708	O	ILE B		89.416 87.475	64.772 66.626	62.428 60.579	1.00	31.62 29.64
	ATOM ATOM	10708	CB CG1			86.180	66.412	59.831		29.14
	ATOM	10710	CG2	ILE B		88.632	66.044	59.715	1.00	31.57
15	ATOM	10711	CD1	ILE B	607	86.001	67.251	58.585	1.00	
	ATOM	10712	N	GLU B		89.277	66.925	63.029		31.23
	ATOM	10713 10714	CA	GLU B		90.602 90.653	66.916 65.920	63.642 64.840		31.09 30.08
	ATOM ATOM	10714	C O	GLU B		91.575	65.100	64.973	1.00	
20	ATOM	10716	ČВ	GLU B		90.978	68.347	63.985	1.00	
	ATOM	10717	CG	GLU B		92.234	68.546	64.831	1.00	36.11
	MOTA	10718	CD	GLU B		93.471	67.991	64.190	1.00	
	MOTA	10719	OE1			93.445	67.821 67.702	62.960 64.929		40.58
25	ATOM ATOM	10720 10721	OE2 N	GLU B ALA B		94.447 89.616	65.907	65.666	1.00	
23	ATOM	10721	CA	ALA B		89.602	65.008	66.815		27.89
	ATOM	10723	C	ALA B		89.757	63.593	66.372	1.00	28.03
	MOTA	10724	0	ALA B		90.522	62.823	66.983	1.00	27.07
20	MOTA	10725	СВ	ALA B		88.332	65.143	67.576	1.00	
30	ATOM ATOM	10726 10727	N CA	ALA B		88.980 89.038	63.224 61.882	65.341 64.796		29.31 30.46
	ATOM	10727	C	ALA B		90.447	61.590	64.239		31.96
	ATOM	10729	ŏ	ALA B		90.983	60.499	64.393		30.76
	ATOM	10730	СВ	ALA B		87.993	61.728	63.725		31.13
35	ATOM	10731	N	ARG B		91.047	62.569	63.576		34.38
	ATOM	10732 10733	CA C	ARG B		92.448 93.359	62.417 62.083	63.173 64.363		36.62 37.55
	ATOM ATOM	10733	0	ARG B		94.146	61.132	64.319	1.00	37.49
	ATOM	10735	ČВ	ARG B		92.975	63.686	62.556		37.15
40	ATOM	10736	CG	ARG B	611	92.409	64.030	61.232		39.17
	ATOM	10737	CD	ARG B		93.246	65.083	60.505		41.10
	ATOM	10738 10739	NE CZ	ARG B		92.638 92.682	65.476 64.741	59.242 58.142	1.00	
	ATOM ATOM	10739		ARG B		93.313	63.552	58.139	1.00	
45	ATOM	10741	NH2	ARG B		92.104	65.195	57.030	1.00	
	MOTA	10742	N	GLN B		93.282	62.871	65.418		38.42
	ATOM	10743	CA	GLN B		94.140	62.595	66.567		39.96
	ATOM	10744	C	GLN B		93.799 94.711	61.266 60.510	67.182 67.554		41.27 42.50
50	ATOM ATOM	10745 10746	O CB	GLN B	612	94.067	63.688	67.613		40.19
30	ATOM	10747	CG	GLN B		94.906	64.871	67.197		40.92
	ATOM	10748	CD	GLN B	612	95.099	65.864	68.276		40.60
	MOTA	10749		GLN B		95.153	65.511	69.446		40.23
c	ATOM	10750	NE2	GLN B		95.204 92.515	67.127 60.923	67.893 67.245		41.14 41.37
55	MOTA MOTA	10751 10752	N CA	PHE B		92.180	59.645	67.835		41.93
	ATOM	10753	C	PHE B		92.852	58.529	67.056		42.81
	ATOM	10754	ō	PHE B		93.341	57.564	67.655	1.00	42.45
	ATOM	10755	CB	PHE B		90.664	59.428	67.915		42.06
60	MOTA	10756	CG	PHE B		89.963	60.342	68.897		40.97
	ATOM	10757 10758		PHE B		90.580 88.675	60.723 60.807	70.086 68.625		39.82 38.60
	MOTA MOTA	10759		PHE B		89.934	61.556	70.977		38.32
	ATOM	10760	CE2	PHE B		88.019	61.621	69.504		37.41
65	ATOM	10761	CZ	PHE B	613	88.649	62.012	70.690	1.00	38.28
	MOTA	10762	N	SER B	614	92.864	58.671	65.732		44.37
	MOTA	10763	CA	SER B		93.507	57.716	64.813		46.26
	MOTA MOTA	10764 10765	C	SER B		94.969 95.479	57.460 56.382	65.102 64.779		47.54 47.97
70	ATOM	10765	CB	SER B	_	93.479	58.219	63.379		46.05
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ATOM
              10767
                       OG
                           SER B 614
                                             92.122
                                                       58.265
                                                                 62.954
                                                                           1.00 47.57
       ATOM
              10768
                      N
                           LYS
                                B 615
                                             95.644
                                                       58.456
                                                                 65.672
                                                                           1.00 48.47
       ATOM
              10769
                                                       58.323
57.757
                                                                 65.981
67.375
                      CA
                           LYS
                                В
                                  615
                                             97.060
                                                                           1.00 49.77
       MOTA
              10770
                      С
                           LYS
                                  615
                                             97.262
                                В
                                                                           1.00
                                                                                49.54
       ATOM
              10771
                                                       57.901
                      0
                           LYS B
                                  615
                                             98.340
                                                                 67.947
                                                                           1.00 50.00
       MOTA
              10772
                                             97.764
97.995
                      CB
                           LYS B 615
                                                       59.679
                                                                           1.00 49.86
                                                                 65.921
      ATOM
              10773
                      CG
                           LYS B
                                  615
                                                       60.231
                                                                 64.539
                                                                          1.00 52.76
      ATOM
              10774
                      CD
                                             99.008
                           LYS B 615
                                                       61.414
                                                                 64.620
                                                                          1.00
                                                                                55.47
      MOTA
              10775
                      CE
                           LYS B 615
                                             98.927
                                                                 63.415
                                                       62.385
                                                                          1.00 56.51
  10
      ATOM
              10776
                      NZ
                           LYS B 615
                                             99.486
                                                       63.757
                                                                 63.735
                                                                          1.00 55.70
              10777
      ATOM
                      N
                                             96.221
                                                       57.200
                           MET B 616
                                                                          1.00
                                                                 67.973
                                                                                49.06
              10778
      MOTA
                      CA
                           MET B 616
                                                                69.284
68.946
                                             96.404
                                                       56.596
                                                                                48.60
                                                                          1.00
      MOTA
                                             96.638
                                                       55.111
              10779
                      С
                           MET B 616
                                                                          1.00
                                                                                47.93
                                                                68.142
70.238
70.751
      MOTA
              10780
                                             95.936
95.213
95.060
                      0
                           MET B 616
                                                       54.482
                                                                          1.00 48.34
 15
      ATOM
              10781
                                                       56.851
                      CB
                           MET B 616
                                                                          1.00 49.16
      MOTA
             10782
                      CG
                           MET B
                                  616
                                                       58.332
                                                                          1.00 49.13
      MOTA
              10783
                      SD
                           MET B 616
                                             93.571
                                                       58.737
                                                                71.827
                                                                          1.00 49.24
      MOTA
             10784
                      CE
                           MET B 616
                                             93.720
                                                                71.881
                                                       60.480
                                                                          1.00 43.96
      MOTA
             10785
                                             97.670
                      N
                           GLY B 617
                                                       54.546
                                                                69.522
                                                                          1.00 46.79
      ATOM
 20
             10786
                      CA
                           GLY B 617
                                             98.040
                                                       53.204
                                                                69.131
                                                                          1.00 45.51
      MOTA
             10787
                           GLY B 617
                      C
                                             96.886
                                                                          1.00 43.75
1.00 43.25
                                                       52.233
                                                                69.138
      ATOM
             10788
                      О
                           GLY B 617
                                             97.038
                                                       51.139
                                                                68.590
      ATOM
             10789
                      N
                           PHE B 618
                                             95.742
                                                      52.621
                                                                69.721
                                                                          1.00 41.77
      ATOM
             10790
                                             94.635
93.398
                      CA
                           PHE B 618
                                                      51.677
                                                                69.889
                                                                          1.00 40.09
 25
      ATOM
             10791
                      С
                           PHE B 618
                                                                68.974
                                                      51.831
                                                                          1.00
                                                                                39.67
      MOTA
             10792
                      0
                           PHE B 618
                                             92.412
                                                      51.092
                                                                69.122
                                                                          1.00 38.13
      ATOM
             10793
                      CB
                           PHE
                               B 618
                                             94.238
93.787
                                                      51.590
                                                                71.361
                                                                          1.00 39.95
             10794
      MOTA
                                                      52.894
53.300
                      CG
                           PHE
                               B 618
                                                                71.975
                                                                          1.00 40.73
      ATOM
             10795
                      CD1 PHE B 618
                                             92.480
                                                                71.882
                                                                          1.00 38.86
 30
      ATOM
             10796
                                                                72.692
72.451
73.272
                     CD2 PHE B 618
                                             94.678
                                                      53.689
                                                                          1.00 42.73
             10797
      ATOM
                                             92.052
                     CE1
                          PHE B 618
                                                      54.469
                                                                          1.00 39.59
             10798
      ATOM
                     CE2
                          PHE
                               В 618
                                             94.261
                                                      54.881
                                                                          1.00 41.95
                          PHE B 618
      ATOM
             10799
                                            92.936
                     CZ
                                                      55.267
                                                                73.161
                                                                          1.00 42.27
     ATOM
             10800
                                            93.429
92.303
                     Ŋ
                          VAL B 619
                                                      52.750
                                                                68.019
                                                                          1.00 39.25
35
     ATOM
             10801
                          VAL B 619
                     CA
                                                      52.791
                                                                67.094
                                                                         1.00 39.86
     ATOM
             10802
                                            92.742
93.769
                     C
                          VAL B 619
                                                      52.435
                                                                65.686
                                                                         1.00 39.43
                          VAL B 619
     ATOM
             10803
                     0
                                                      52.868
                                                                65.199
                                                                         1.00 39.46
1.00 39.76
     MOTA
             10804
                     CB
                                            91.497
91.676
                          VAL B 619
                                                      54.087
                                                                67.092
                                                      54.839
54.915
     ATOM
             10805
                     CG1
                          VAL B 619
                                                                68.343
65.930
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5	ATOM ATOM ATOM	10980 10981 10982	O N CA	GLY B SER B SER B	642 642	82.051 82.873 84.017	67.295 66.316 67.187	51.696 53.560 53.620	1.00 29.05 1.00 29.53 1.00 29.91
10	ATOM ATOM ATOM	10983 10984 10985	C O CB	SER B SER B	642 642	85.170 85.976 84.582	66.768 67.607 67.206	52.678 52.287 55.028	1.00 31.18 1.00 31.66 1.00 29.68
10	ATOM ATOM ATOM	10986 10987 10988 10989	OG N CA C	SER B GLY B GLY B	643 643	85.219 85.259 86.341 87.582	65.956 65.483 64.941 64.561	55.281 52.364 51.565 52.375	1.00 28.01 1.00 32.16 1.00 33.04 1.00 33.77
15	ATOM ATOM ATOM	10990 10991 10992	O N CA	GLY B SER B SER B	643 644	88.597 87.463 88.615	64.215 64.579 64.404	51.814 53.695 54.595	1.00 33.62 1.00 34.07 1.00 34.04
20	ATOM ATOM	10993 10994 10995	C O CB	SER B SER B	644 644	89.333 90.552 88.167	63.079 62.990 64.519	54.409 54.610 56.076	1.00 34.10 1.00 34.02 1.00 33.03
20	ATOM ATOM ATOM	10996 10997 10998 10999	OG N CA C	SER B GLY B GLY B	645 645	87.585 88.569 89.112 89.207	63.294 62.047 60.707 59.961	56.498 54.075 53.898 55.203	1.00 31.58 1.00 34.16 1.00 33.94 1.00 34.82
25	ATOM ATOM ATOM	11000 11001 11002	O N CA	GLY B VAL B VAL B	645 646 646	89.521 88.917 89.080	58.765 60.647 60.025	55.245 56.300 57.605	1.00 35.73 1.00 34.33 1.00 33.90
30	ATOM ATOM ATOM	11003 11004 11005 11006	C O CB	VAL B VAL B VAL B	646 646	87.989 88.235 89.111 89.123	59.008 58.021 61.129 60.546	57.932 58.615 58.672 60.086	1.00 33.16 1.00 32.54 1.00 34.58 1.00 34.63
30	ATOM ATOM ATOM	11008 11008 11009	CG1 CG2 N CA		646 647	90.338 86.780 85.668	62.054 59.217 58.345	58.407 57.433 57.828	1.00 34.03 1.00 34.31 1.00 32.43 1.00 32.12
35	ATOM ATOM ATOM	11010 11011 11012	C O CB	PHE B PHE B PHE B	647 647 647	85.239 85.004 84.484	57.394 57.789 59.215	56.756 55.670 58.241	1.00 31.73 1.00 32.31 1.00 32.01
40	ATOM ATOM ATOM	11013 11014 11015	CD2	PHE B PHE B	647 647	84.819 85.398 84.561	60.173 61.391 59.863	59.325 59.037 60.643	1.00 31.30 1.00 31.77 1.00 31.08
40	ATOM ATOM ATOM ATOM	11016 11017 11018 11019	CE1 CE2 CZ N	PHE B PHE B PHE B LYS B	647 647	85.716 84.894 85.477 85.096	62.284 60.754 61.944 56.127	60.066 61.656 61.353 57.090	1.00 28.09 1.00 28.81 1.00 27.39 1.00 32.24
45	ATOM ATOM ATOM	11020 11021 11022	CA C O	LYS B LYS B LYS B	648 648 648	84.673 83.168 82.679	55.125 55.162 54.875	56.138 55.964 54.897	1.00 31.64 1.00 32.05 1.00 30.31
50	ATOM ATOM ATOM	11023 11024 11025	CD	LYS B LYS B	648 648	85.045 84.533 85.342	53.751 52.555 51.367	56.660 55.852 56.257	1.00 32.05 1.00 31.04 1.00 32.31
50	ATOM ATOM ATOM ATOM	11026 11027 11028 11029	CE NZ N CA	LYS B LYS B CYS B	648 649	84.668 84.285 82.422 80.966	50.064 49.810 55.500 55.524	56.104 54.731 57.013 56.893	1.00 35.71 1.00 39.53 1.00 31.54 1.00 32.41
55	ATOM ATOM ATOM	11030 11031 11032	C O CB	CYS B CYS B CYS B	649 649	80.289 80.907 80.428	56.334 56.668 54.118	57.988 58.967 56.967	1.00 31.12 1.00 30.91 1.00 32.74
	ATOM ATOM ATOM	11033 11034 11035	SG N CA	CYS B GLY B GLY B	650 650	80.676 79.015 78.238	53.369 56.663 57.378	58.582 57.789 58.787	1.00 37.84 1.00 30.42 1.00 29.72
60	ATOM ATOM	11036 11037 11038	C O N	GLY B GLY B ILE B	650 651	76.727 76.193 76.055	57.321 56.973 57.697	58.638 57.571 59.731	1.00 28.44 1.00 27.80 1.00 26.95
65	ATOM ATOM ATOM	11039 11040 11041 11042	CA C O CB	ILE B ILE B ILE B	651 651	74.614 74.102 74.453 74.137	57.677 59.005 59.425 56.626	59.821 60.319 61.392 60.817	1.00 25.90 1.00 25.19 1.00 24.71 1.00 25.72
	ATOM ATOM ATOM	11042 11043 11044 11045	CG1	ILE B	651 651	74.768 72.594 74.579	55.285 56.507 54.338	60.574 60.774 61.740	1.00 24.38 1.00 26.85 1.00 26.43
70	ATOM	11046	N	ALA B		73.254	59.651	59.538	1.00 24.38

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	ATOM ATOM ATOM	11117 11118 11119	N CA C	TYR	В	661 661 661	(64. 64.	745 596 227	75.931 75.073 75.006	56.172 56.481 57.960	1.00	24.04 23.76 23.19
5	ATOM ATOM ATOM ATOM	11120 11121 11122 11123	O CB CG	TYR TYR	B B	661 661	(64. 65.	156 844 054 499	74.455 73.629 73.451 74.306	58.326 56.023 54.570 53.638	1.00	23.04 24.22 23.41 25.96
10	ATOM ATOM ATOM	11124 11125 11126		TYR TYR	B B	661 661	(65. 64.	813 750 026	72.391 74.139 72.195	54.102 52.255 52.733	1.00 1.00	28.26 24.48 26.73
	ATOM ATOM ATOM	11127 11128 11129	CZ OH N	TYR TYR TYR	B B	661 662	. (65.° 65.	500 727 093 879	73.078 72.842 75.552	51.826 50.473 58.817	1.00	27.30 31.51 22.68
15	ATOM ATOM ATOM ATOM	11130 11131 11132 11133	CA C O CB	TYR TYR TYR TYR	B B	662 662	(54.: 53.:	879 161 988 164	75.452 76.652 77.668 75.072	60.256 60.890 60.239 60.980	1.00	22.16 22.58 21.76 22.02
20	ATOM ATOM ATOM	11134 11135 11136	CG CD1 CD2	TYR TYR TYR	B B B	662 662 662	6	55.6 56.3	387	74.449 73.388 74.967	62.325 62.411 63.495	1.00 1.00 1.00	21.48 21.91 23.40
	ATOM ATOM ATOM	11137 11138 11139 11140	CE1 CE2 CZ OH	TYR TYR TYR TYR	B B	662 662	6	66.0 65.2	649 054 174 801	72.838 74.383 73.322 72.662	63.607 64.770 64.797 65.959	1.00 1.00	22.92 24.30 24.12 19.23
25	ATOM ATOM ATOM	11141 11142 11143	N CA C	ASP ASP ASP	B B B	663 663	6	53.6 52.8 53.6	669 882 660	76.493 77.560 78.860	62.123 62.761 63.030	1.00 1.00 1.00	22.74 24.01 24.75
30	ATOM ATOM ATOM	11144 11145 11146 11147	O CB CG	ASP ASP ASP	B B	663 663	6	54.8 52.8 52.8	075 895	78.873 77.087 76.808 77.721	63.182 63.970 65.212 65.839	1.00	24.67 23.36 24.97 21.98
	ATOM ATOM ATOM	11148 11149 11150		ASP SER SER	B B	663 664	6	52.8 52.9 53.9	889 919	75.668 79.956 81.272	65.707 63.000 63.135	1.00	27.41 25.55 26.43
35	ATOM ATOM ATOM	11151 11152 11153	C O CB	SER SER SER	B B	664 664	6	54.2 55.3 52.4	350 452	81.495 81.982 82.368	64.431 64.430 62.995 63.911	1.00	26.07 26.65 26.25 25.95
40	ATOM ATOM ATOM ATOM	11154 11155 11156 11157	OG N CA C	SER VAL VAL VAL	B B B	665 665 665	6 6	51.4 53.5 54.1 55.5	599 180 531	82.164 81.167 81.466 80.820	65.543 66.822 67.018	1.00 1.00 1.00	25.54 25.02 25.27
45	ATOM ATOM ATOM	11158 11159 11160 11161		VAL VAL VAL	B B	665 665	6	6.4 3.2 3.8	250 397	81.471 81.065 81.417 81.772	67.493 68.007 69.407 67.909	1.00 1.00	25.08 25.18 24.49 24.54
43	ATOM ATOM ATOM	11162 11163 11164	N CA C	TYR TYR TYR	B B	666 666	6	55.6 56.8	540	79.528 78.828 79.252	66.709 66.941 65.928	1.00 1.00 1.00	24.73 23.57 24.38
50	ATOM ATOM ATOM ATOM	11165 11166 11167 11168	O CB CG	TYR TYR TYR TYR	B B	666 666	6	9.0 6.6 7.9	597 994	79.527 77.316 76.469 76.288	66.308 66.900 67.056 65.993	1.00	24.18 23.24 21.71 22.85
55	ATOM ATOM ATOM	11169 11170 11171	CD2 CE1	TYR TYR TYR	B B	666 666	6	8.3 9.9	300 985	75.864 75.538 75.074	68.254 66.098 68.414	1.00 1.00	25.29 25.06 27.49
	ATOM ATOM	11172 11173 11174	CZ OH N	TYR TYR THR	B B	666 667	7 6	0.3 1.4 7.5	121 532	74.934 74.186 79.343	67.322 67.419 64.658	1.00 1.00	27.05 27.36 24.04
60	ATOM ATOM ATOM ATOM	11175 11176 11177 11178	CA C O CB	THR THR THR	B B	667 667	6 7	8 . 5 9 . 0 10 . 3)97 315	79.562 80.944 81.104 79.313	63.599 63.584 63.493 62.258	1.00 1.00	24.34 25.40 24.23 25.25
65	ATOM ATOM ATOM	11179 11180 11181	OG1 CG2 N	THR THR GLU	B B B	667 667 668	6 6 6	7.2 8.8 8.2	267 376 217	78.003 79.340 81.940	62.248 61.107 63.678	1.00 1.00 1.00	25.15 23.81 26.00
	ATOM ATOM ATOM ATOM	11182 11183 11184 11185	CA C O CB	GLU GLU GLU	B B	668 668	. 7	8 . 6 9 . 4 0 . 3 7 . 4	186 377	83.324 83.675 84.522 84.233	63.599 64.817 64.740 63.498	1.00 1.00	26.42 27.19 27.51 25.94
70	ATOM	11186	CG	GLU				6.5		83.896	62.243		27.24

	ATOM ATOM ATOM	11188 11189	OE2	L GLU 2 GLU	B	668 668 669	65 64	5.231 5.018 4.380 9.252	85.479 84.162	63.0)66 394	1.00) 29) 30	.27
5	ATOM ATOM ATOM ATOM	11191 11192 11193	CA C O	ARG ARG	B B B	669 669 669	70 71 72	0.044 L.528 2.339	83.287 83.126 83.880	67.1 66.8 67.3	101 310 335	1.00 1.00 1.00 1.00) 27) 27) 27	.00 .41 .58 .79
10	ATOM ATOM ATOM ATOM	11195 11196 11197	CG CD NE CZ	ARG ARG ARG ARG	B B B	669 669 669	70 69 69).552).894).815).708	82.687 82.262	69.5 70.7 70.8	99 353	1.00 1.00 1.00) 28) 30) 32	.52 .22 .37
15	ATOM ATOM ATOM ATOM	11200 11201 11202	NH1 NH2 N CA	ARG ARG TYR TYR	B B B	669 669 670 670	67 68 71 73	7.505 8.835 877 8.256	80.610 78.762 82.106 81.851	70.7 70.8 66.0 65.6	36 75 31 78	1.00 1.00 1.00	32 32 28 28	.60 .35 .01 .42
20	ATOM ATOM ATOM ATOM	11204 11205 11206	C O CB CG	TYR TYR TYR TYR	B B	670 670 670	74 73 73	.632 .809 .569	82.365 82.531 80.351 79.710	63.9 65.7	80 33	1.00 1.00 1.00	28 28	.53 .12
	ATOM ATOM ATOM ATOM	11208 11209 11210	CD1 CD2 CE1 CE2	TYR TYR TYR	B B B	670 670 670	71 73	.635 .918 .130 .416	79.983 78.904 79.450 78.344	68.2 66.9 69.3 68.1	71 94	1.00 1.00 1.00	27 29	. 11 . 84
25	ATOM ATOM ATOM ATOM	11211 11212 11213 11214	CZ OH N CA	TYR TYR MET MET	B B	670 671	71 72	.029 .533 .667	78.622 78.119 82.625 82.882	69.3 70.5 63.4 62.0	12 31	1.00 1.00 1.00	27 28 30	.33 .94 .33
30	ATOM ATOM ATOM ATOM	11215 11216 11217 11218	C O CB CG	MET MET MET MET	B 6 B 6	671	72 72 72	.600 .901 .442	84.235 84.586 81.795 80.414	61.5 60.3 61.1	36 92 32	1.00 1.00 1.00	31. 30. 30.	06 69 61
35	ATOM ATOM ATOM ATOM	11219 11220 11221 11222	SD CE N CA	MET MET GLY GLY	B 6 B 6 B 6	671 671 672 672	74 73 71 71	.640 .905 .831	80.253 80.430 84.952 86.197	60.25 58.66 62.33	54 01 36	1.00 1.00 1.00 1.00	30. 32. 31.	11 95 71
40	ATOM ATOM ATOM	11223 11224 11225 11226	C O N CA	GLY GLY LEU LEU	B 6 B 6	572 573 573	69 69	.160 .617 .854 .852	85.871 84.779 86.820 86.643	60.86 60.87 59.98 58.94	70 33	1.00 1.00 1.00 1.00	32. 32. 33.	93 80 57
	ATOM ATOM ATOM ATOM	11227 11228 11229 11230	C CB CG	LEU LEU LEU	В 6 В 6	573 573	70 68	.450 .515 .112 .448	86.222 86.694 87.956 88.500	57.62 57.21 58.74 60.01	L8 11	1.00 1.00 1.00	33. 34.	95 73
45	ATOM ATOM ATOM ATOM	11231 11232 11233 11234		LEU LEU PRO PRO	В 6 В 6	573 574	66. 68	.879 .362 .749 .217	89.870 87.532 85.352	59.76 60.41 56.90	54 L7)3	1.00 1.00 1.00	36. 36. 37.	42 99 00
50	ATOM ATOM ATOM ATOM	11235 11236 11237 11238	C O CB CG	PRO PRO PRO PRO	В 6 В 6	74 74	68 68 68	.829 .021 .464 .139	85.963 85.646 83.635 84.010	54.52 53.64 55.42 55.93	28 15 25	1.00 1.00 1.00 1.00	40. 39. 37.	15 73 86
55	ATOM ATOM ATOM ATOM ATOM	11239 11240 11241 11242 11243	CD N CA	PRO THR THR THR	B 6 B 6 B 6	74 75 75 75	67. 69. 69. 70.	477 366 218 611	84.689 87.182 88.225 88.638	57.22 54.64 53.62 53.14	6	1.00 1.00 1.00 1.00	37. 41. 43. 43.	42 47 02 72
60	ATOM ATOM ATOM ATOM	11244 11245 11246 11247	CB OG1 CG2	THR I	B 6 B 6 B 6	75 75 75	68. 69. 67.	604 479 224 126 700	88.445 89.477 90.066 89.136 89.191	53.85 54.16 55.24 54.78 51.93	3 7	1.00 1.00 1.00 1.00	43.3 45.3 43.3	15 83 20
65	ATOM ATOM ATOM ATOM	11248 11249 11250 11251	CA C O	PRO I PRO I PRO I PRO I	B 6 B 6 B 6	76 76 76	71. 72. 73.	991 603 800 591	89.634 90.713 90.838 90.231	51.38 52.25 52.43 50.01	0 6 9	1.00 1.00 1.00	44.3 43.9 43.6	30 57 54
	ATOM ATOM ATOM ATOM	11252 11253 11254 11255	CD N CA	PRO I PRO I GLU I GLU I	3 6°	76 77	69. 71. 71.	307 588 701 973	89.548 89.428 91.491 92.572	49.68 51.00 52.79 53.70	5 0 8	1.00 1.00 1.00	44.5 44.5 43.6	53 58 57
70	ATOM	11256	C	GLU E	3 6	77	72.	621	92.019	54.98		1.00		

	ATOM	11257	0	GLU	В	677	73	.256	92.771	55.728	1.00	43.51
	ATOM	11258	CB	GLU			70	. 625	93.245	54.036	1.00	44.76
	ATOM	11259	CG	GLU	В	677		.575	93.052	52.916	1.00	47.36
	ATOM	11260	CD	GLU	В	677	68	.135	93.125	53.392	1.00	51.20
5	ATOM	11261	OE1	GLU	В	677	67	.866	93.836	54.381	1.00	54.53
	ATOM	11262	OE2		В	677	67	.256	92.479	52.770	1.00	54.13
	ATOM	11263	N	ASP				.482	90.720	55.251	1.00	41.72
	ATOM	11264	CA	ASP	В	678	73	.013	90.185	56.502	1.00	40.99
	ATOM	11265	С	ASP	В	678	73	.846	88.917	56.341	1.00	39.07
10	MOTA	11266	0	ASP	В	678	75	.044	88.986	56.074	1.00	37.79
•	ATOM	11267	CB	ASP	В	678	71	.882	89.992	57.538	1.00	41.34
	ATOM	11268	CG	ASP	В	678	72	.413	89.618	58.936	1.00	42.84
	ATOM	11269	OD1	ASP	В	678	73	.628	89.707	59.162	1.00	46.59
	ATOM	11270	OD2	ASP	В	678	71	.699	89.210	59.868	1.00	45.40
15	ATOM	11271	N	ASN	В	679	73	.240	87.751	56.491	1.00	37.03
	ATOM	11272	CA	ASN	В	679	74	.061	86.561	56.470	1.00	36.29
	ATOM	11273	С	ASN	В	679	73	.701	85.502	55.435	1.00	35.66
	ATOM	11274	0	ASN	\mathbf{B}	679	74	.024	84.344	55.623	1.00	35.59
	MOTA	11275	CB	ASN	В	679		.112	85.966	57.888	1.00	35.38
20	ATOM	11276	CG	ASN	В	679	75	.315	85.076	58.093	1.00	35.81
	ATOM	11277	OD1	ASN	В	679	75	.271	84.065	58.829	1.00	36.44
	ATOM	11278	ND2	ASN	В	679	76	.407	85.429	57.426	1.00	30.49
	ATOM	11279	N	LEU	В	680	73	.074	85.893	54.330		36.18
	ATOM	11280	CA	LEU	В	680	72	.665	84.940	53.282		37.04
25	ATOM	11281	С	LEU	В	680		.759	84.052	52.745		37.17
	ATOM	11282	0	LEU	В	680		.558	82.845	52.559		37.42
	ATOM	11283	CB	LEU	В	680	72	.076	85.664	52.075		37.58
	ATOM	11284	CG	LEU		680		.958	85.022	51.240		39.69
	ATOM	11285		LEU		680		.226	85.257	49.772		41.11
30	ATOM	11286	CD2	LEU		680		.729	83.532	51.484		40.41
	MOTA	11287	N	ASP		681		.926	84.623	52.483		37.50
	ATOM	11288	CA	ASP		681		.964	83.855	51.830		38.01
	ATOM	11289	С	ASP		681		.345	82.586	52.632		37.14
	ATOM	11290	0	ASP		681		. 483	81.483	52.065		36.38
35	ATOM	11291	CB.	ASP		681		.199	84.722	51.515		39.14
	ATOM	11292	CG	ASP		681		.887	85.920	50.571		43.26
	ATOM	11293		ASP		681		.109	85.762	49.609		46.71
	ATOM	11294		ASP		681		.384	87.070	50.723		48.74
40	ATOM	11295	N	HIS		682		.568	82.742	53.929		35.59 35.67
40	ATOM	11296	CA	HIS		682		.893	81.582	54.738 54.930		33.61
	ATOM	11297	C	HIS		682 682		.673 .867	80.632 79.452	55.143		33.15
	MOTA	11298	O	HIS HIS		682		.524	81.927	56.099		35.65
	MOTA	11299 11300	CB CG	HIS		682		.040	80.714	56.806		37.66
45	ATOM ATOM	11300		HIS		682		.298	80.030	57.750		37.90
43	ATOM	11301	CD2			682		.190	80.012	56.659		38.17
	ATOM	11302		HIS				.969	78.967	58.159		31.97
	ATOM	11303		HIS				.123	78.935	57.518		37.82
	ATOM	11305	N	TYR				.448	81.149	54.879		32.10
50	ATOM	11306	CA	TYR	В	683	73	.285	80.257	54.857		31.92
	ATOM	11307	C	TYR				.414	79.342	53.630		31.93
	ATOM	11308	ō	TYR			73	.244	78.158	53.724		28.90
	ATOM	11309	СВ	TYR				.986	81.044	54.770		31.15
	ATOM	11310	CG	TYR	В	683		.275	81.405	56.071		30.21
55	ATOM	11311	CD1	TYR				.535	82.598	56.716	1.00	29.38
	ATOM	11312	CD2	TYR				.290	80.571	56.619	1.00	28.21
	ATOM	11313	CE1	TYR		683		. 866	82.965	57.828	1.00	27.01
	ATOM	11314	CE2	TYR		683	69	.611	80.935	57.728	1.00	27.18
	ATOM	11315	CZ	TYR	В	683	69	. 905	82.136	58.339		27.90
60	ATOM	11316	OH	TYR	В	683	69	.254	82.523	59.472		27.60
	ATOM	11317	N	ARG	В	684	73	. 825	79.909	52.490		33.70
	ATOM	11318	CA	ARG	В	684	73	. 958	79.138	51.231		33.97
	ATOM	11319	С	ARG	В	684	75	.188	78.258	51.116	1.00	33.32
	ATOM	11320	0	ARG			75	.154	77.247	50.441		31.95
65	ATOM	11321	СВ	ARG		684		. 975	80.080	50.031		35.11
	MOTA	11322	CG	ARG		684		. 642	80.274	49.422		39.47
	MOTA	11323	CD	ARG				.744	80.970	50.302		42.04
	MOTA	11324	NE	ARG	В	684		.290	80.772	50.137		45.44
	MOTA	11325	CZ	ARG				.535	81.284	49.182		45.72
70	MOTA	11326	NH1	ARG	В	684	70	. 057	81.935	48.153	1.00	46.39

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	ATOM	11417	0_	LYS			82.193	57.220	47.250		36.72
	ATOM ATOM	11418 11419	CB CG	LYS LYS		696	81.296 82.562	59.492 60.245	45.223 44.839		37.25 40.92
	ATOM	11419	CD	LYS			82.355	61.033	43.490		44.08
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25	ATOM	11430		GLN			87.581 85.929	61.288 62.783	49.275 48.843		49.24
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	ATOM	11433	CA	VAL			81.760	57.191	51.967		31.84
	MOTA	11434	C	VAL			80.462	56.400	51.846		31.25
	MOTA	11435	0	VAL			79.782	56.489	50.826		30.83
40	MOTA	11436	CB	VAL			81.539	58.324	52.958 53.216		31.73
	ATOM ATOM	11437 11438		VAL VAL			82.813 80.491	59.102 59.258	52.452		32.77
	ATOM	11439	N N	GLU			80.145	55.598	52.869		30.04
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55	ATOM	11451	Ö	TYR			73.997	55.657	53.418		24.19
55	ATOM	11452	ČВ	TYR			75.764	58.238	53.352		26.07
	ATOM	11453	CG	TYR			74.997	59.418	53.933		24.42
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	ATOM	11458	CZ	TYR			73.685	61.683	54.807		24.01
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65	ATOM	11461	CA	LEU			72.740	56.002	55.958		23.60
	ATOM	11462	C	LEU LEU		701	72.050 72.565	57.268 57.992	56.454 57.353		23.98 23.64
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70	ATOM	11466		LEU			70.344	54.071	56.500	1.00	26.22

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-	ATOM AOTA				68.759	· -	56.525	1.00 22.87
-	AOTA (702 702	68.089			
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	ATOM	11517	OD2 ASP B 7		62.319	65.109	62.642	1.00 17.00
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	ATOM	11520	C ASP B 7		57.170 58.278	68.793 69.756	62.954 63.284	1.00 22.26
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5	ATOM ATOM	11680 11681	O CB		в 73 В 73		73.443	57.234	50.115	1.00	27.96
	ATOM	11682	CG		В 73		72.176	57.823	49.561	1.00	29.42
	ATOM	11683	CD1		в 73	0	72.127	58.314	48.280	1.00	30.54
	ATOM	11684	CD2				71.033	57.899	50.342	1.00	33.30
10	ATOM	11685	CE1	PHE			70.953	58.860	47.749	1.00	32.34
10	ATOM	11686	CE2	PHE PHE			69.851 69.818	58.448 58.931	49.834 48.532	1.00	33.34 33.29
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	ATOM	11689	CA	GLN			71.275	53.904	52.066	1.00	29.87
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	ATOM	11699	С	ALA :			66.951	54.520	54.129	1.00	29.27
o.=	ATOM	11700	0_	ALA			66.761	53.313	53.925	1.00	
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	ATOM ATOM	11702	N CA		3 73. 3 73.		65.145	54.760	55.769	1.00	
	ATOM	11704	C		3 73		64.260	55.891	56.248	1.00	
	ATOM	11705	O		3 73		64.706	56.747	57.047	1.00	24.40
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	ATOM	11707	CG	MET I			65.317	52.628	56.979	1.00	35.13
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35	ATOM	11711	CA		3 73		62.025	56.798	56.369		24.63
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45	ATOM ATOM	11721 11722	CZ2 CZ3	TRP I			58.567 60.641	53.718 54.373	52.762 51.670	1.00	22.58 26.40
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55	ATOM	11731	CD2	TYR I			62.821	55.419	60.816		22.29
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	ATOM	11733	CE2	TYR I			63.789	54.421	60.900		23.07
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60	ATOM ATOM	11736	N	THR I			57.578	56.044	58.983		21.77
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65	ATOM	11741		THR E			55.776	55.010 55.727	56.905		22.43 23.21
	ATOM ATOM	11742 11743	N CG2	THR I			53.894 55.118	55.727 58.250	58.053 60.005		22.73
	ATOM	11743	CA	ASP I			54.381	58.891	61.080		23.45
	ATOM	11745	C	ASP I	3 73	7	55.175	59.113	62.351		23.50
70	MOTA	11746	0	ASP I			54.566	59.442	63.404	1.00	22.54

5	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	11748 11749 11750 11751 11752	CG OD1 OD2 N CA	ASE ASE GLU GLU	B B B	737 737 737 738 738	53.109 52.019 52.066 51.008 56.492 57.325	58.161 59.048 57.404 58.933 59.187	60.388 59.485 60.432 62.279 63.444	1.0 1.0 1.0 1.0	0 21.91 0 27.05 0 22.71 0 23.28
10	ATOM ATOM ATOM ATOM ATOM	11754 11755 11756 11757 11758		GLU GLU GLU		738 738 738 738 738	57.791 57.944 58.519 58.146 57.587 58.195	61.229 58.243 56.794 56.626 57.140	62.352 63.512 63.843 65.263 66.255	1.00 1.00 1.00 1.00	21.96 23.38 25.58 29.05
15	ATOM ATOM ATOM ATOM ATOM ATOM	11760 11761 11762 11763	OE2 N CA C O CB	ASP ASP ASP	B 7 B 7 B 7	739 739 739 739	56.522 58.000 58.505 60.036	61.181 62.562 62.685 61.738	65.394 64.625 64.722 64.963 64.656	1.00 1.00 1.00	22.43 23.17 22.55 24.43
20	ATOM ATOM ATOM ATOM	11765 11766 11767 11768	CG OD1 OD2 N	HIS	B 7 B 7 B 7	739 739 739 740	57.659 57.844 58.765 57.033 60.521	62.961 62.204 63.378	-65.715 67.117 67.507 67.957 65.428	1.00 1.00 1.00 1.00	20.29
25	ATOM ATOM ATOM ATOM ATOM	11769 11770 11771 11772 11773	CA C O CB CG	HIS HIS HIS HIS	B 7 B 7 B 7	40 40 40	61.938 62.535 63.739 62.219 63.588	64.043 63.036 62.760 65.451 65.974	65.752 66.723 66.661 66.306	1.00 1.00 1.00	22.65 23.57 24.38 22.48
30	ATOM ATOM ATOM ATOM ATOM	11774 11775 11776 11777 11778	ND1 CD2 CE1	HIS HIS HIS GLY	B 7 B 7 B 7 B 7	40 40 40 40	64.131 64.504 65.356 65.594 61.745	65.894 66.632 66.408 66.884 62.477	64.711 66.738 64.730 65.946 67.629	1.00	24.01 21.78 23.93 21.27
35	ATOM ATOM ATOM ATOM ATOM	11779 11780 11781 11782 11783	CA C O N CA	GLY GLY GLY ILE ILE	B 7 B 7 B 7	41 41 42	62.324 62.381 63.160 61.616 61.440	61.524 60.115 59.294 59.840 58.455	68.557 68.020 68.501 66.975 66.513	1.00 1.00 1.00	24.01 23.93 24.35 24.05 24.15
40	ATOM ATOM ATOM ATOM ATOM	11784 11785 11786 11787 11788		ILE ILE ILE ILE	B 7 B 7 B 7	42 42 42	61.389 62.127 62.558 62.716 62.244	57.569 56.591 57.994 58.966 56.614	67.742 67.829 65.565 64.413 64.979	1.00 1.00 1.00 1.00	24.36 24.69
45	ATOM ATOM ATOM ATOM ATOM	11789 11790 11791 11792 11793	CD1 N CA C	ILE ALA ALA ALA ALA	B 74 B 74 B 74 B 74	42 43 43 43	63.908 60.512 60.485 59.398	58.768 57.915 57.274 56.284	63.510 68.677 70.001 70.291	1.00 1.00 1.00 1.00	25.20 24.91 26.61 27.02
50	ATOM ATOM ATOM ATOM ATOM	11794 11795 11796 11797 11798	CB N CA C	ALA SER SER SER SER	B 74 B 74 B 74 B 74	43 44 44 44 44	59.448 60.500 58.441 57.478 58.303 59.344	55.645 58.327 56.084 55.042 53.793 53.594	71.345 71.115 69.393 69.692 69.935 69.336	1.00 1.00 1.00 1.00	
55	ATOM ATOM ATOM ATOM ATOM	11799 11800 11801 11802 11803	OG N CA C	SER SER SER SER SER	B 74 B 74 B 74 B 74	14 15 15 15	56.464 57.078 57.784 58.516 59.004	54.810 54.249 52.919 51.748 50.887	68.563 67.405 70.771 71.161 69.974	1.00 1.00 1.00 1.00	26.67 31.26 28.75 30.40 29.85
60	ATOM ATOM ATOM ATOM ATOM	11804 11805 11806 11807 11808	CB OG N CA	SER SER SER IHR IHR	B 74 B 74 B 74 B 74	15 15 16	60.137 57.677 58.337 58.182 58.630	50.424 50.909 49.672 50.675 49.790	69.986 72.112 72.256 68.946 67.847	1.00 1.00 1.00	29.98 30.34 34.56 29.65 28.90
65	ATOM ATOM ATOM ATOM	11809 11810 11811 11812 11813	O 2 CB 2 OG1 2 CG2 2	THR THR THR THR THR	B 74 B 74 B 74 B 74	6 6 6	59.582 60.524 57.451 56.540 56.651	50.487 49.895 49.234 50.295 48.232	66.901 66.385 67.068 66.707 67.942	1.00 1.00 1.00 1.00	27.78 27.10 29.68 27.85 30.75
70	ATOM ATOM ATOM	11814 11815 11816	CA A	ALA I ALA I	B 74	7	59.364 60.298 61.675	51.760 52.413 52.509	66.645 65.734 66.400	1.00 1.00	27.53

	ATOM ATOM ATOM ATOM	11817 11818 11819 11820	O CB N CA	ALA ALA HIS HIS	B B	747		62.724 59.797 61.673 62.934	52.320 53.754 52.753 52.897	65.745 65.327 67.716 68.463		
5	ATOM ATOM ATOM	11821 11822 11823	C O CB	HIS HIS HIS	B B	748 748 748		63.734 64.953 62.669	51.610 51.637 53.226 53.220	68.350 68.076 69.931 70.794	1.00	27.05 25.75 27.44
10	ATOM ATOM ATOM ATOM ATOM	11824 11825 11826 11827 11828	CD2 CE1	HIS HIS HIS HIS	B B	748 748 748		63.885 64.797 64.321 65.763 65.498	54.244 52.338 53.987 52.836	70.794 70.785 71.725 71.657 72.241	1.00 1.00 1.00	26.51
15	ATOM ATOM ATOM ATOM	11829 11830 11831 11832	N CA C	GLN GLN GLN GLN	B B B	749 749 749		63.059 63.789 64.280 65.369	50.470 49.190 48.984 48.472	68.510 68.399 66.968 66.678	1.00 1.00 1.00	27.15 28.01 27.20 26.40
20	ATOM ATOM ATOM ATOM	11833 11834 11835 11836	CB CG CD OE1	GLN GLN GLN GLN	B B B	749 749 749		62.896 62.459 61.433 61.787	48.020 48.107 47.043 45.894	68.842 70.299 70.712 70.922	1.00 1.00 1.00 1.00	28.88 30.75 35.63 41.39
	ATOM ATOM ATOM ATOM	11837 11838 11839 11840	NE2 N CA C	GLN HIS HIS HIS	B B B	750	1	60.184 63.443 63.721 64.890	47.440 49.404 49.167 50.052	70.862 66.055 64.681 64.227	1.00 1.00 1.00	37.11 27.01 27.01 25.80
25	ATOM ATOM ATOM ATOM	11841 11842 11843 11844		HIS HIS	B B B	750	!	65.794 62.441 62.555 61.614	49.546 49.327 48.845 48.022	63.602 63.860 62.451 61.876	1.00 1.00 1.00	25.66 27.22 28.98 34.83
30	ATOM ATOM ATOM ATOM	11845 11846 11847 11848	CE1	HIS HIS HIS ILE	B B	750 750 750 751	(63.489 61.968 63.099 64.915	49.055 47.748 48.366 51.331	61.506 60.635 60.383 64.584	1.00 1.00 1.00	28.49 31.78 27.98 24.75
35	ATOM ATOM ATOM	11849 11850 11851 11852	CA C O CB	ILE ILE ILE	B B	751 751 751 751	(55.981 57.350 58.305 55.711	52.202 51.745 51.572 53.688	64.630 63.858 64.305	1.00 1.00	24.56 24.17 23.48 23.55
40	ATOM ATOM ATOM ATOM	11853 11854 11855 11856	CG1 CG2 CD1 N	ILE ILE TYR	B B	751 751 751 752	(56.729 55.814 56.537 57.435	54.493 54.070 55.999 51.461	63.524 65.770 63.550 65.922	1.00 1.00	25.42 26.58 25.36 23.88
	ATOM ATOM ATOM ATOM	11857 11858 11859 11860	CA C O CB	TYR TYR TYR TYR	B B	752 752 752 752		58.716 59.152 70.356 58.696	51.006 49.642 49.341 51.033	66.471 65.939 65.864 68.016	1.00 1.00	23.89 24.36 24.86 23.90
45	ATOM ATOM ATOM ATOM	11861 11862 11863 11864	CG CD1 CD2 CE1	TYR TYR TYR	B B B	752 752 752	((58.908 70.202 57.820 70.406	52.438 52.985 53.256	68.505 68.564 68.841 69.001	1.00 1.00 1.00	23.39 21.30 21.53 19.82
50	ATOM ATOM ATOM ATOM	11865 11866 11867 11868		TYR TYR TYR THR	B B B	752 752 752	6	58.023 59.322 59.504 58.190	54.584 55.069 56.353 48.823	69.216 69.328 69.701 65.545	1.00 1.00 1.00	22.84 22.05 26.93 24.72
55	ATOM ATOM ATOM ATOM	11869 11870 11871 11872	CA C O CB	THR THR THR THR	B B B	753 753 753	6	58.499 59.130 70.055 57.254	47.540 47.719 46.986 46.686	64.949 63.599 63.227 64.821	1.00 1.00 1.00	25.04 25.21 25.42 25.19
60	ATOM ATOM ATOM ATOM	11873 11874 11875		THR	B B B	753 753 754	6	66.815 57.552 58.591 58.992	46.327 45.322 48.676 48.934	66.129 64.189 62.859 61.509	1.00 1.00 1.00	26.51 26.77 25.43 24.78
50	ATOM ATOM ATOM	11876 11877 11878 11879	C O CB	HIS HIS	B B B	754 754 754		70.363 71.207 58.031	49.549 49.166 49.899	61.526 60.769 60.832	1.00 1.00 1.00	24.51 23.52 24.32
65	ATOM ATOM ATOM	11880 11881 11882 11883	CD2 CE1	HIS HIS HIS	B B B	754 754 754	6	58.090 57.869 58.269 57.960	49.863 48.707 50.852 48.982	59.336 58.609 58.428 57.319	1.00 1.00 1.00	23.90 23.25 24.23 21.88
70	ATOM ATOM ATOM	11884 11885 11886	NE2 N CA	HIS MET MET	В	755	7	58.190 70.577 71.887	50.276 50.512 51.163	57.180 62.407 62.511	1.00	23.11 25.06 24.45

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ATOM
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                      C
                           MET B 755
                                            72.973
                                                      50.195
                                                               63.052
                                                                        1.00 24.60
       MOTA
              11888
                      0
                                  755
                                            74.151
                           MET
                               В
                                                      50.335
                                                               62.717
                                                                        1.00 22.03
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                                            71.789
                               В
                                                               63.426
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       ATOM
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                      CG
                           MET
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                                            70.852
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72.583
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                           SER B 756
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       MOTA
              11894
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                           SER B 756
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                                                                        1.00
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                                                     47.471
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      ATOM
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                                 756
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                                                     47.388
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             11897
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                          SER B 756
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                                                     47.385
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             11898
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                          HIS B 757
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                                                               62.430
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                                                                              27.68
                          HIS B 757
HIS B 757
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      MOTA
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                     CE1 HIS.B 757
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                                                              61.784
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             11909
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                          PHE B
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      ATOM
             11911
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                          PHE B 758
                                           76.286
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      ATOM
             11912
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74.221
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                          PHE B
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                                                     49.055
                                                              59.003
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      MOTA
             11913
                     CB
                          PHE B 758
                                                     50.499
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                                                                        1.00 27.19
      ATOM
             11914
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                          PHE B 758
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                          PHE B 758
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             11916
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                          PHE
                              B 758
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75.372
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      MOTA
                     CE1 PHE
                              В
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     ATOM
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                         PHE B
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1.00 28.75
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                          PHE B 758
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                                                              56.465
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77.723
78.505
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     ATOM
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                          ILE B
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                                                                       1.00 30.09
     ATOM
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                          ILE B
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     ATOM
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     MOTA
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                                759
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77.290
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50.584
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            11926
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78.582
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                         LYS
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45.764
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                         LYS
                              В
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                         LYS B
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1.00 35.22
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77.221
77.344
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                         LYS B
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                         LYS
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45.970
45.690
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78.845
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80.897
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                         GLN B 761
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46.909
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56.935
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                         GLN B 761
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    MOTA
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                    С
                         CYS B 762
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    ATOM
                    CB
                        CYS
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65
    ATOM
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                    SG
                        CYS B
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           11952
    ATOM
                    N
                         PHE B 763
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                                                                            38.96
    ATOM
           11953
                    CA
                         PHE
                             В
                               763
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           11954
    ATOM
                    С
                         PHE
                             В
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                                                                      1.00 40.32
    ATOM
           11955
                               763
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                        PHE
                             В
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                                                                      1.00 39.92
                                                             61.015
70
    ATOM
           11956
                    CB
                        PHE B 763
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                                                   47.807
                                                             61.868
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5	ATOM ATOM ATOM ATOM ATOM	11957 11958 11959 11960 11961 11962	CG CD1 CD2 CE1 CE2 CZ	PHE PHE	B 7 B 7 B 7 B 7	63 63 63 63	83.038 83.606 82.584 83.702 82.673 83.227	5 50 1 49 2 51 3 51	273 2211 2.692 2.517 2.020	61.423 63.488 61.819 63.878	1.00 1.00 1.00 1.00	35.95 34.28 36.76 33.55 33.00 32.46
10	ATOM ATOM ATOM ATOM ATOM	11963 11964 11965 11966 11967 11968	N CA C O CB OG	SER SER SER SER SER	B 7 B 7 B 7 B 7	64 64 64 64	83.060 83.281 83.192 84.038 84.631	43 2 43 3 42 43 44	320 8.895 9.024 9.145 9.677	59.036 60.284 60.498 58.354 57.279	1.00 1.00 1.00 1.00	41.75 42.70 44.33 45.27 42.68 40.08
15	ATOM ATOM ATOM ATOM ATOM ATOM	11969 11970 11971 11972 11973 11974	N CA C O CB CG	LEU LEU LEU LEU LEU	B 7 B 7 B 7 B 7	65 65 65 65	82.167 81.891 80.703 79.635 81.550	42 41 42 43	.263 .461 .527 .000 .373	62.264 61.982 61.626 63.450	1.00 1.00 1.00 1.00	45.12 46.20 47.52 47.72 46.04 46.16
20	ATOM ATOM ATOM ATOM ATOM	11975 11976 11977 11978 11979	CD1 CD2 N CA C	LEU LEU PRO PRO PRO	3 7 3 7 3 7 3 7	65 65 66 66	82.184 83.787 80.873 79.765 78.590	45 43 40 39	.259 .424 .212 .261 .490	64.996 64.619 62.143 61.948 62.907	1.00 1.00 1.00 1.00	46.29 46.53 48.72 49.30 49.42
25	ATOM ATOM ATOM ATOM TER	11980 11981 11982 11983 11984 M11985	O CB CG CD	PRO : PRO : PRO : PRO : PRO : NAG :	3 7 3 7 3 7 3 7	66 66 66 66	78.756 80.407 81.831 82.124	37 38 39	.282 .899 .101 .517		1.00 1.00 1.00	49.18 49.19 49.63 49.18
30	HETATI HETATI HETATI HETATI	M11986 M11987 M11988 M11989 M11990	C2 N2 C7 O7 C8	NAG I NAG I NAG I NAG I NAG I	3 7: 3 7: 3 7: 3 7:	93 93 93 93	32.573 32.577 33.128 33.450 33.376	65 66 66 67	.000 .287 .514 .654	78.742 79.402 80.598 80.963 81.538	1.00 1.00 1.00 1.00	61.12 61.79 63.53 65.37 63.95
35	HETATI HETATI HETATI	M11991 M11992 M11993 M11994 M11995	C3 O3 C4 O4 C5	NAG I NAG I NAG I NAG I	3 7: 3 7: 3 7: 3 7:	93 93 93 93	31.628 30.285 31.723 30.728 33.122	64 62 61 62	.988 .421 .749 .837 .160	79.397 79.591 78.530 78.927 78.732	1.00 1.00 1.00 1.00	63.28 61.99 63.93 62.43 64.92
40	HETATI HETATI HETATI HETATI	M11996 M11997 M11998 M11999 M12000	C6 O6 O5 C1 C2	NAG I NAG I NAG I NAG I	3 75 3 75 3 75 3 75	93 93 94 94	33.290 34.269 34.179 55.667 54.300	61 63 62 62	.932 .217 .069 .444 .821	77.842 76.867 78.445 110.980 110.434	1.00 1.00 1.00 1.00	60.71 34.19 34.04
45	HETATI HETATI HETATI HETATI	M12001 M12002 M12003 M12004 M12005	C3	NAG I NAG I NAG I NAG I	3 79 3 79 3 79	94 94 94 94	54.500 54.026 53.459 54.215 53.760	62 61 63 64	.246 .012	109.054 108.007 108.025 106.719 111.199	1.00 1.00 1.00 1.00	32.45 30.69 29.04 28.12 35.55
50	HETATI HETATI HETATI HETATI	M12006 M12007 M12008 M12009 M12010		NAG I NAG I NAG I NAG I	3 79 3 79 3 79 3 79	94 94 94 94	52.487 53.648 53.272 55.010 54.946	63 64 63 62	.653 .805 .195 .678	110.702 112.679 113.391 113.177 114.607	1.00 1.00 1.00 1.00	40.00 36.40 34.43 32.95 33.12
55	HETATI HETATI HETATI HETATI	M12012 M12013 M12014 M12015	C2 N2	NAG I NAG I NAG I NAG I	3 79 3 79 3 79	94 96 96 96	53.967 55.494 46.134 45.064 44.194	62 89 90 89	.672 .146 .074 .053	114.764 112.353 64.573 65.068 66.099	1.00 1.00 1.00 1.00	28.48 35.51 37.06 39.18 38.69
60	HETATI HETATI HETATI HETATI	M12017 M12018 M12019 M12020	O7 C8 C3 O3	NAG I NAG I NAG I NAG I	3 79 3 79 3 79 3 79	96 96 96 96	44.254 45.136 43.179 44.162 43.318	90 89 90 91	.894 .611 .381 .454 .468	67.359 67.793 68.270 63.915 64.403	1.00 1.00 1.00 1.00	41.45 45.89 41.70 40.21 39.86
65	HETATI HETATI HETATI HETATI	M12022 M12023 M12024	O4 C5 C6	NAG I NAG I NAG I NAG I	3 79 3 79 3 79	96 96 96	44.987 44.302 46.322 47.244 47.617	90 90 91	.975 .814 .248 .170	62.748 61.526 62.597 61.831 60.756	1.00 1.00 1.00	43.50 44.51 43.28 43.03 44.68
70	HETATI			NAG I			46.961	89	. 876	63.806	1.00	36.35

	HETATM12027 HETATM12028 HETATM12029	C2	NAG NAG	B 797 B 797 B 797	49.268 49.691 48.733	48.602	96.293	1.00 62.31
5	HETATM12030 HETATM12031 HETATM12032 HETATM12033	. 07 C8	NAG NAG	B 797 B 797 B 797	48.798 49.868 47.463	48.715 48.995 48.951	94.079 93.512 93.439	1.00 63.61 1.00 61.06 1.00 64.40
10	HETATM12034 HETATM12035	03 C4	NAG NAG	B 797 B 797 B 797 B 797	49.905 50.543 50.776 51.162	46.394 47.922	96.566 98.392	1.00 60.47 1.00 61.34
•	HETATM12037 HETATM12038 HETATM12039 HETATM12040	C6 06	NAG NAG	B 797 B 797 B 797 B 797	49.921 50.437 51.831	48.982 49.402 49.550	99.073 100.454 100.437	1.00 61.24 1.00 60.99 1.00 58.34
15	HETATM12041 HETATM12042 HETATM12043	0 0 0	нон нон нон	1 2 4	49.878 69.755 39.998 62.220	80.399 46.901 40.486	86.643 18.457 27.246	1.00 61.78 1.00 7.73 1.00 10.31 1.00 12.87
20	HETATM12044 HETATM12045 HETATM12046 HETATM12047	0 0 0	НОН НОН НОН НОН	5 6 7 8	64.826 56.767 50.245 78.281	36.556 35.394 56.483	36.335	1.00 19.31 1.00 21.00 1.00 20.14 1.00 37.18
25	HETATM12048 HETATM12049 HETATM12050 HETATM12051	0 0 0	НОН НОН НОН НОН	9 10 11 12	56.125 36.083 59.581 34.041	73.117 37.083 32.583 50.937	69.619 46.767 52.936	1.00 19.38 1.00 39.78 1.00 27.38
	HETATM12052 HETATM12053 HETATM12054	0 0 0	НОН НОН НОН	13 14 15	65.320 31.494 62.642	47.187 58.838 72.239	39.008 62.009 35.693 59.850	1.00 20.61 1.00 24.23 1.00 22.60 1.00 23.18
30	HETATM12055 HETATM12056 HETATM12057 HETATM12058	0 0 0	НОН НОН НОН НОН	16 17 18 19	77.995 58.533 88.208 40.525	58.866 67.745 29.565 72.824	78.221 55.662 21.093 73.221	1.00 15.42 1.00 22.30 1.00 49.26 1.00 21.32
35	HETATM12059 HETATM12060 HETATM12061	0 0 0	нон нон	20 21 22	48.198 73.384 50.583	59.827 76.365 31.754	34.355 48.426 30.128	1.00 25.55 1.00 33.50 1.00 27.05
	HETATM12062 HETATM12063 HETATM12064 HETATM12065	000	HOH HOH HOH HOH	23 24 25 26	31.043 52.509 36.878 65.794	56.428 59.981 45.981 61.426	38.581 46.771 19.156 46.509	1.00 23.41 1.00 25.42 1.00 26.52 1.00 22.37
40	HETATM12066 HETATM12067 HETATM12068	0 0	нон нон	27 28 29	50.084 54.775 80.149	61.646 55.861 72.731	50.977 63.543 69.030	1.00 25.11 1.00 31.76 1.00 22.40
45	HETATM12069 HETATM12070 HETATM12071 HETATM12072	0 0 0	НОН НОН НОН НОН	30 31 32 33	27.782 74.208 82.869 80.923	60.784 56.149 57.914 58.743	35.598 72.170 96.204 73.558	1.00 29.54 1.00 19.00 1.00 32.13 1.00 27.31
50	HETATM12073 HETATM12074 HETATM12075 HETATM12076	0 0 0	нон нон	34 35 36	55.022 69.840 30.001	78.846 71.834 58.932	65.695 89.800 39.011	1.00 26.47 1.00 22.74 1.00 25.83
30	HETATM12077 HETATM12078 HETATM12079	0 0 0	НОН НОН НОН НОН	37 38 39 40	62.208 57.842 37.983 52.081	61.143 52.910 42.872 75.115	103.510 58.684 24.658 70.879	1.00 37.15 1.00 23.27 1.00 20.62 1.00 26.06
55	HETATM12080 HETATM12081 HETATM12082 HETATM12083	0 0 0	НОН НОН НОН	41 42 43	72.496 73.302 43.663	54.302 69.745 65.019	43.326 86.804 34.139	1.00 32.87 1.00 26.45 1.00 23.93
60	HETATM12084 HETATM12085 HETATM12086	0000	нон нон нон	44 45 46 48	66.893 56.462 58.082 25.975	48.699 68.617 66.385 61.038	89.087 53.861 58.226 32.629	1.00 30.37 1.00 24.87 1.00 23.90 1.00 27.79
	HETATM12087 HETATM12088 HETATM12089	0 0 0	нон нон нон	49 50 51	34.089 82.210 29.874	59.708 91.526 69.711	48.959 102.461 84.012	1.00 28.45 1.00 41.43 1.00 35.20
65	HETATM12090 HETATM12091 HETATM12092 HETATM12093	0000	НОН НОН НОН НОН	52 53 54 55	83.150 43.509 38.606 51.005	70.002 44.094 76.598 36.317	67.331 56.593 91.780 35.795	1.00 33.57 1.00 32.63 1.00 30.60
70	HETATM12094 HETATM12095 HETATM12096	0 0	нон нон нон	56 57 58	70.432 35.211 81.995	83.664 69.922 70.997	85.676 74.499 89.633	1.00 39.38 1.00 26.32 1.00 37.11 1.00 28.50

	HETATM12097	0	нон	59	50.463	38.807		1.00 39.80
	HETATM12098	0	нон	60	47.949	31.885		1.00 22.69
	HETATM12099 HETATM12100	0	нон нон	61 62	47.182 60.983	54.781 33.345		1.00 20.23 1.00 28.58
5	HETATM12101	ő	нон	63	65.450	85.673		1.00 28.30
,	HETATM12102	ŏ	нон	64	62.565	62.304		1.00 16.92
	HETATM12103	ŏ	нон	65	61.679	72.418		1.00 24.32
	HETATM12104	0	HOH	66	79.506	66.115	69.527	1.00 26.96
	HETATM12105	0	HOH	68	54.535	64.150		1.00 19.13
10	HETATM12106	0	нон	69	60.608	52.351		1.00 22.94
	HETATM12107	0	НОН	70 72	51.046 56.903	59.344		1.00 22.26 1.00 21.85
	HETATM12108 HETATM12109	0	НОН НОН	73	50.482	55.928 56.281		1.00 21.83
	HETATM12109	ŏ	НОН	74	83.719	69.898		1.00 24.14
15	HETATM12111	ŏ	НОН	75	79.910	80.755		1.00 24.86
	HETATM12112	0	HOH	76	57.730	71.048	70.318	1.00 22.20
	HETATM12113	0	HOH	77	65.844	87.314	99.634	1.00 23.32
	HETATM12114	0	HOH	78	73.533	63.176	68.120	1.00 17.04
20	HETATM12115	0	HOH	79 80	82.010 57.970	77.243 68.804	76.246 68.829	1.00 23.87 1.00 19.26
20	HETATM12116 HETATM12117	0	НОН НОН	81	81.575	64.030	69.005	1.00 19.20
	HETATM12117	ŏ	нон	82	64.683	44.537	33.113	1.00 24.42
	HETATM12119	ŏ	нон	83	46.606	55.961	55.295	1.00 22.83
	HETATM12120	0	HOH	84	52.899	58.974	38.346	1.00 18.29
25	HETATM12121	0	HOH	85	73.770	82.389	80.349	1.00 21.67
	HETATM12122	0	нон	86	44.010	34.967	29.064	1.00 26.14
	HETATM12123	0	HOH	87 88	58.796	62.203 52.744	38.296 34.980	1.00 38.76 1.00 34.59
	HETATM12124 HETATM12125	0	нон нон	89	52.117 57.055	44.447	37.217	1.00 34.39
30	HETATM12126	ŏ	НОН	90	51.256	34.490	38.049	1.00 33.84
	HETATM12127	ō	нон	91	46.866	25.435	39.522	1.00 46.43
	HETATM12128	0	нон	92	46.232	22.556	41.496	1.00 42.39
	HETATM12129	0	нон	93	59.548	45.139	35.000	1.00 42.25
35	HETATM12130	0	HOH	94	62.857	46.175	65.622	1.00 19.05
55	HETATM12131 HETATM12132	0	НОН НОН	95 96	55.251 67.380	51.600 57.546	69.221 70.835	1.00 24.07 1.00 28.58
	HETATM12132	0	НОН	97	70.645	58.099	73:586	1.00 20.58
	HETATM12134	ŏ	нон	98	74.810	58.797	72.603	1.00 27.25
	HETATM12135	0	HOH	99	77.511	55.043	76.924	1.00 26.31
40	HETATM12136	0	HOH	100	60.609	64.994	69.994	1.00 34.49
	HETATM12137	0	НОН	101	61.574	66.028	75.139	1.00 31.31
	HETATM12138 HETATM12139	0	НОН НОН	102 103	68.125 93.361	68.933 75.876	71.197 61.155	1.00 32.38 1.00 50.17
	HETATM12139	0	HOH	103	92.339	75.801	77.524	1.00 30.17
45	HETATM12141	ŏ	нон	105	89.509	76.668	77.238	1.00 36.60
	HETATM12142	Ō	нон	106	96.453	75.594	77.314	1.00 34.90
	HETATM12143	0	нон	107	83.581	63.013	51.557	1.00 28.63
	HETATM12144	0	нон	108	76.910	56.310	50.467	1.00 28.57
50	HETATM12145	0	HOH	109	88.046	54.771	55.131	1.00 44.11 1.00 33.60
50	HETATM12146 HETATM12147	0	НОН НОН	110 111	80.838 81.869	89.466 77.174	77.925 92.013	1.00 33.00
	HETATM12148	ŏ	нон	112	85.641	73.512	93.741	1.00 26.83
	HETATM12149	ŏ	нон	113	88.338	80.641	90.398	1.00 40.73
	HETATM12150	0	HOH	114	72.839	75.180	103.334	1.00 31.56
55	HETATM12151	0	НОН	115	76.390	64.819	106.832	1.00 32.74
	HETATM12152	0	нон	116	70.062		104.604	1.00 34.31 1.00 38.13
	HETATM12153 HETATM12154	0	нон нон	117 118	67.748 68.759	54.004 50.320	101.069 98.367	1.00 57.66
	HETATM12155	ŏ	нон	119	84.379	38.809	82.154	1.00 36.63
60	HETATM12156	ŏ	НОН	120	73.754	50.392	47.910	1.00 21.15
	HETATM12157	0	HOH	121	78.379	46.740	34.934	1.00 24.31
	HETATM12158	0	HOH	122	63.544	35.488	9.380	1.00 31.34
	HETATM12159	0	НОН	123	44.179	34.979	13.105	1.00 25.61
65	HETATM12160 HETATM12161	0	нон нон	124 125	52.909 50.961	50.685 44.497	14.735 18.295	1.00 34.54 1.00 23.10
05	HETATM12161	0	HOH	125	36.677	57.474	22.449	1.00 23.10
	HETATM12163	ŏ	нон	127	41.507	53.667	24.386	1.00 51.04
	HETATM12164	ŏ	нон	128	27.040	64.555	5.523	1.00 39.18
	HETATM12165	0	нон	129	20.081	69.745	25.535	1.00 36.99
70	HETATM12166	0	нон	130	22.434	70.829	16.822	1.00 37.46

		HETATM1216	7 0	нон	131	41.88	4 83.942	26.261	. 1.00 44.34
		HETATM1216	8 0	нон	132	39.86	6 65.248		
		HETATM1216		HOH	133	36.72			1.00 37.09
	5	HETATM12170		НОН НОН	134 135	62.59 63.09			
		HETATM1217		НОН	136	66.99			
		HETATM12173	_	НОН	137	63.82	5 76.390		
		HETATM12174 HETATM12175		HOH	138	57.55		81.797	1.00 49.39
	10			НОН НОН	139 140	51.43 50.91		87.594 92.867	
		HETATM12177	_	нон	141	53.63		74.968	
		HETATM12178	_	нон	142	59.14	2 88.533	56.693	1.00 40.75
		HETATM12179 HETATM12180		нон нон	143 144	58.55		50.505	
	15	HETATM12181	_	НОН	144	67.61 53.90		44.131 47.344	
		HETATM12182	. 0	НОН	146	53.79		-3.567	1.00 43.67
		HETATM12183		НОН	147	64.23		24.925	1.00 33.58
		HETATM12184 HETATM12185		НОН НОН	148 202	66.49	_	47.228	1.00 29.81
	20	HETATM12186	Ö	НОН	202	32.619 43.839		51.879 49.564	1.00 30.37 1.00 28.20
		HETATM12187		нон	206	37.580	57.461	52.650	1.00 27.92
		HETATM12188		HOH	208	42.183		55.700	1.00 34.76
		HETATM12189 HETATM12190		нон нон	210 212	39.538 48.96		54.332	1.00 25.41
	25	HETATM12191		нон	214	71.887		65.352 75.646	1.00 44.84 1.00 28.47
		HETATM12192	0	HOH	216	71.427	55.779	72.292	1.00 35.84
		HETATM12193 HETATM12194	0	НОН НОН	· 218 220	70.822		77.949	1.00 30.76
		HETATM12195	ŏ	HOH	222	69.998 71.248		78.356 79.600	1.00 22.45 1.00 38.95
	30	HETATM12196	Ò	нон	224	56.680		88.555	1.00 38.93
		HETATM12197	0	нон	226	57.373		86.390	1.00 49.30
		HETATM12198 HETATM12199	0	нон нон	228 230	75.894 75.429		74.472	1.00 28.54
		HETATM12200	ŏ	нон	232	56.996		66.254 55.734	1.00 48.76 1.00 33.84
	35	HETATM12201	0	HOH	234	64.723	80.578	51.996	1.00 38.72
		HETATM12202 HETATM12203	0	НОН НОН	236	51.212		54.717	1.00 25.78
		HETATM12204	Ö	HOH	238 240	48.051 41.990		66.773 71.279	1.00 29.08 1.00 32.98
		HETATM12205	Ō	НОН	242	39.086	89.203	74.974	1.00 32.98
	40	HETATM12206	0	нон	244	81.152	36.150	29.584	1.00 33.69
		HETATM12207 HETATM12208	0	НОН НОН	245 246	78.600 51.499	49.867 59.265	34.219	1.00 26.08
	45	HETATM12209	ŏ	нон	247	46.560	55.997	-6.134 30.696	1.00 34.07 1.00 26.99
		HETATM12210	0	HOH	248	51.695	64.028	29.990	1.00 23.45
		HETATM12211 HETATM12212	0	HOH	249	50.152	59.677	36.121	1.00 27.45
		HETATM12213	0	нон нон	250 251	53.824 52.542	56.732 60.702	35.090 34.717	1.00 31.08 1.00 33.68
		HETATM12214	ŏ	НОН	252	57.043	64.788	39.705	1.00 33.68
	50	HETATM12215	0	НОН	253	54.472	63.858	40.439	1.00 29.74
	50	HETATM12216 HETATM12217	0	нон нон	254 255	47.192 42.136	45.492	35.067	1.00 38.53
		HETATM12218	ŏ	НОН	256	48.624	51.046 43.656	33.979 28.724	1.00 37.48 1.00 35.99
		HETATM12219	0	HOH	257	53.099	40.645	24.972	1.00 24.40
	55	HETATM12220 HETATM12221	0	HOH	258	49.300	44.995	31.514	1.00 35.06
	33	HETATM12221	0	НОН НОН	259 260	46.593 44.469	49.097	33.004	1.00 45.88
		HETATM12223	ŏ	НОН	261	41.442	49.208 46.842	32.906 26.549	1.00 39.68 1.00 26.59
	60	HETATM12224	0	HOH	262	43.277	51.017	31.045	1.00 40.35
		HETATM12225	0	НОН	263	39.106	54.477	24.710	1.00 57.23
		HETATM12226 HETATM12227	0	нон нон	264 265	40.193 43.286	61.253	24.178	1.00 27.83
		HETATM12228	ŏ	нон	266	35.232	61.838 59.526	21.847 15.974	1.00 47.16
		HETATM12229	ŏ	нон	267	38.799	65.129	17.277	1.00 33.54 1.00 32.63
	4 5	HETATM12230	0	нон	268	45.335	68.698	15.891	1.00 39.70
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	70	HETATM12235	0	нон	273	34.907	79.293	33.911	1.00 38.34
	70	HETATM12236	0	нон	274	45.725	61.512	35.273	1.00 22.54

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	C. I. C. III				

Column 2 lists a number for the atom in the structure.

Column 3 lists the element whose coordinates are measured. The first letter in the column defines 65 the element.

Column 4 lists the type of amino acid.
Column 5 lists a number for the amino acid in the structure.

Columns 6-8 list the crystallographic coordinates X, Y, and Z respectively. The crystallographic coordinates define the atomic position of the element measured.

Column 9 lists an occupancy factor that refers to the fraction of the molecules in which each atom occupies the position specified by the coordinates. A value of "1" indicates that each atom has the same conformation, i. e., the same position, in all molecules of the crystal.

Column 10 lists a thermal factor "B" that measures movement of the atom around its atomic

center.

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Claims

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- 1. A crystal of the extracellular domain of mammalian DPP-IV.
- 2. The crystal of claim 1, characterized as having an orthorhombic space group of $P2_12_12_1$ and one homodimer of DPP-IV in the asymmetric unit.
- The crystal of claims 1 and 2, wherein the crystal has unit cell dimensions of:
 a is from 63 Å to 70 Å;
 b is from 66 Å to 70 Å;
 c is from 416 Å to 424 Å;
 and a P2₁2₁2₁ symmetry.
- 4. The crystal of claims 1 to 3, characterized by the atomic structure coordinates of Table 4.
 - 5. A co-crystal of the extracellular domain of mammalian DPP-IV and a ligand bound to its active site.
 - 6. The crystal of claim 5, characterized as having an orthorhombic space group of $P2_12_12_1$ and one homodimer of DPP-IV in the asymmetric unit.
 - 7. The co-crystal of claim 6, wherein the co-crystal has unit cell dimensions of:

 a is from 63 Å to 70 Å;
 b is from 66 Å to 70 Å;
 c is from 416 Å to 424 Å;
 and a P2₁2₁2₁ symmetry.
 - 8. A co-crystal of the extracellular domain of mammalian DPP-IV and a ligand bound to an allosteric binding site.
 - 9. A co-crystal of the extracellular domain of mammalian DPP-IV and HgCl₂.
 - 10. A method for crystallizing mammalian DPP-IV, the method comprising

 (a) providing a buffered, aqueous solution of pH 7 to 8.5 with a concentration of 7 mg/ml to 22 mg/ml of the extracellular domain of mammalian DPP-IV; and

 (b) growing crystals by vapor diffusion using a buffered reservoir solution with between 10% and 30% PEG, between 10% and 20% glycerol, wherein PEG has an average molecular weight between 1000 and 20000.

11. The method according to claim 10, wherein the extracellular domain of mammalian DPP-IV of step (a) is produced in P. pastoris and then deglycosylated.

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- 12. A method for co-crystallizing mammalian DPP-IV and an active site ligand, the method comprising
 - (a) providing a buffered, aqueous solution of pH 7 to 8.5 with a concentration of 7 mg/ml to 22 mg/ml of the extracellular domain of mammalian DPP-IV;
 - (b) adding a molar excess of the active site ligand to the aqueous solution of mammalian DPP-IV;
 - (c) growing crystals by vapor diffusion using a buffered reservoir solution with between 10% and 30% PEG, between 10% and 20% glycerol, wherein PEG has an average molecular weight between 1000 and 20000.
- 13. The method according to claim 12, wherein the extracellular domain of mammalian DPP-IV of step (a) is produced in P. pastoris and then deglycosylated.
- 14. A crystal produced by the methods according to claims 10 to 13.
- 15. A method for determining the three-dimensional structure of a crystallized extracellular domain of mammalian DPP-IV to a resolution of 3.5Å to 2.1Å or better, the method comprising
 - (a) crystallizing an extracellular domain of mammalian DPP-IV; and
 (b) analysing the extracellular domain of mammalian DPP-IV by X-ray
 diffraction to determine the three-dimensional structure of the crystallized
 extracellular domain of mammalian DPP-IV, whereby the three-dimensional
 structure of a crystallized extracellular domain of mammalian DPP-IV is
 determined to a resolution of 3.5Å to 2.1Å or better.
- 16. A machine-readable data storage medium comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, displays a graphical three-dimensional representation of a molecule or molecular complex comprising at least a portion of the extracellular domain of mammalian DPP-IV comprising the amino acids of SEQ ID NO:2, the extracellular domain comprising the ligand binding active site being defined by a set of points having a root mean square deviation of less than about 1.5Å from points representing the backbone atoms of said amino acids as represented by structure coordinates listed in Table 4.

- 17. A method for identifying a compound that interacts with DPP-IV, comprising the steps of
 - (a) generating a three-dimensional model of DPP-IV using the structure coordinates listed in Table 4, a root mean square deviation from the backbone atoms of said amino acids of less than 1.5Å; and
 - (b) employing said three-dimensional model to design or select a compound that interacts with DPP-IV.
- 18. The method according to claim 17, further comprising the steps of
 - (c) obtaining the identified compound; and

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- (d) contacting the obtained compound with DPP-IV in order to determine the effect the compound has on DPP-IV activity.
- 19. The method according to claims 17 and 18, wherein the compound interacts with the active site of DPP-IV.
- 20. The method according to claims 17 and 18, wherein the compound interacts with an allosteric binding site of DPP-IV.
- 21. The method according to claims 17 and 20, wherein the compound is an inhibitor of DPP-IV activity.
- 22. The method according to claims 17 to 21, wherein the method is a computer-assisted method.
- 23. A compound identified by the methods according to claims 17 to 22.
 - 24. A pharmaceutical composition comprising the compound of claim 23 and a pharmaceutically acceptable carrier.
 - 25. A compound according to claim 23 for use as a therapeutic active substance, in particular for the treatment of diabetes type I, diabetes type II, IGT, obesity and cancer.
 - 26. An isolated nucleic acid sequence encoding the soluble extracellular domain of DPP-IV comprising the nucleotide sequence of SEQ ID NO:1.
 - 27. A nucleic acid construct comprising an expression vector and the nucleic acid sequence according to claim 26.
- 28. A host cell transformed with the nucleic acid construct according to claim 27.

- 29. A method of producing the soluble extracellular domain of DPP-IV comprising culturing the host cell of claim 28 under conditions permitting the expression of the soluble extracellular domain of DPP-IV by the host cell.
- 30. The method according to claim 29, wherein the host cell is P. pastoris.
- 5 31. A polypeptide comprising the soluble extracellular domain of DPP-IV as set forth in SEQ ID NO:2.

- 32. Use of a compound according to claim 23 for the manufacture of a medicament for the treatment of diabetes type-I, diabetes type-II, IGT, obesity and cancer.
- 33. Use of a crystal or a co-crystal according to claims 1 to 9 for the identification and/or design of inhibitors of DPP-IV activity.
- 34. The novel crystals, methods, compounds, compositions and uses substantially as herein before described especially with reference to the foregoing Examples.

Abstract

The present invention relates to crystal structure information obtained from crystals of the dipeptidyl-peptidase DPP-IV, to methods of preparing such crystals, and to their use for the identification and/or design of inhibitors of DPP-IV activity. A further subject matter of the invention are methods for the identification and/or design of inhibitor compounds of DPP-IV activity, the inhibitor compounds of DPP-IV activity identified by these methods and their use in pharmaceutical compositions for the treatment and/or prevention of diseases comprising diabetes types I and II, IGT, obesity and cancer.

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Figure 1

			transmembrane area .L al*	
	hDPPIV	1	MKTPWKWALE LEGICAL VIEW TWEWWALNKGTDDATADSRKTYTLTDYLK 5	0
	rDPPIV	1		
5			β1/1 β1/2 β1/3 ∨ β1/4	
			Y Part	
	hDPPIV	51	NTYRLKLYSLRWISDHEYLYKQENNILVFNAEYGNSSVFLENSTFDEFGH 1	
	rDPPIV	49	F-V-SVST,HIEID 9	8
10			$\beta 2/1$ $\beta 2/2$ $\beta 2/2$ $\beta 2/2$ $\beta 2/3$ $\beta 2/4$	
10	hDPPIV	101	SINDYSISPDGQFILLEYNYVKQWRHSYTASYDIYDLNKRQLITEERIPN 1	Ε Λ
	rDPPIV		SVRL-V	
				=0
			β3/1 β3/2 β3/3 β3/4 β3/4 a	
15	hDPPIV	151	NTQWVTWSPVGHKLAYVWNNDIYVKIEPNLPSYRITWTGKEDIIYNGITD 20	00
	rDPPIV	149	IQEKHHSNV-FN- 19	98
			α2* 84(1 94/2) 81*	
			D4/1 D4/2	
20	hDPPIV			50
20	rDPPIV	199	I-G	48
			β2*	
	hDPPIV	251		20
	rDPPIV		WIVTT 29	
25				
			B5/1 β5/2 β5/3 β5/4h	
	hDPPIV		CDV:TWATQER:SDOWLRRIQNYSVMDICDYDE WNC WNC PAR ON I 35	
	rDPPIV	299	A-VSEDAKTTLVPTTQET-A 34	18
			9612	
30	hDPPIV	251	86'1 86/2 86/3 85'4	_
	rDPPIV		TGWVGRFRPSEPHFTLDGNSFYKIISNEEGYRHICYFQIDKKDCTFI 39CASSV-DKDKQK-R-PEQV 39	
	IDEFIV	Jaj		78
			β7/1 β7/2 β7/3 β7/4	
35	hDPPIV	398	TKGTWEVIGIEALTSDYLYYISNEYKGMPGGRNLYKIQLSDYTKVTCLSC 44	17
	rDPPIV		ASEET-H-NKK 44	
	•			
			β8/1 β8/2 β8/3 β8/4	
40			ELNPERCQYYSVSFSKEAKYYQLRCSGPGLPLYTLHSSVNDKGLRVLEDN 49	
40	rDPPIV	449	DR-TDQ-E 49	8
			α4* β1 β2 β3	
	hDPPIV	498	SALDKMLQNVQMPSKKLDFIIL.NETKFWYQMILPPHFDKSKKYPLLLDV 54	_
	rDPPIV			
45	POP	430	KGIDASDYQTVQIFYPSKDGTKIPMFTVHKKGIKLDGSHPAFT.YG 47	
			· · ·	_
			αΑ β4 αΒ'	
	hDPPIV	547	AGPCSQKADTVFRL.NwallasteniivasfdGRGsGyQGDKIMHAI. 59	4
	rDPPIV		AA 59	5
50	POP	473	GGFNISI TOMVCVSRLIFVRHMCCVT MIMITRGCCFVCFTWHKGGI 51	9
			αB β5' β5 αC	

	hDPPIV	595	NRRLGTFEVEDQIEAARQFSKMGFVDNKRIAIWGWYGGYVTSMVLGSGS 6	4.
	rDPPIV	596	77 T	4
	POP	520	LAN.KONCFDDFQCAAEYLIKEGYTSPKRLTINGGENGGLLVATCANQRP 5	
5			8-S- with C762 and	
	hDPPIV	645	GVFKCGIAVAPVSRWEYYDSVIIIIXYMGLPTPEDNLDHYRNSTVM 6	89
	rDPPIV	646		90
	POP	569	DLFGCVIAQVGVMDMIKEHKYTIGHAWTTDYG.CSDSKOHFEWLIKYSPL 6	17
10			β7	
	hDPPIV	690	SRAENFKQVEYLLIHGTA DNVHFQQSAQISKALVDVGV 72	27
	rDPPIV	691	A 72	
	POP	618	HNVKLPEADDIQYPSMLLLTADHEDRVVPLHSLKFIATLQYIVGRSRKQN 66	
15			β8 αF -S-S- with C649	
	hDPPIV	728	.DFQAMWYTDED G.IASSTAHQHIYTHMSHFIKQCFSLP 766	
	rDPPIV	729	·R 767	
	POP	668	NPLLIHVDTKAG GAGKPTAKVIEEVSDMFAFIARCLNIDWIP 710	

Figure 2

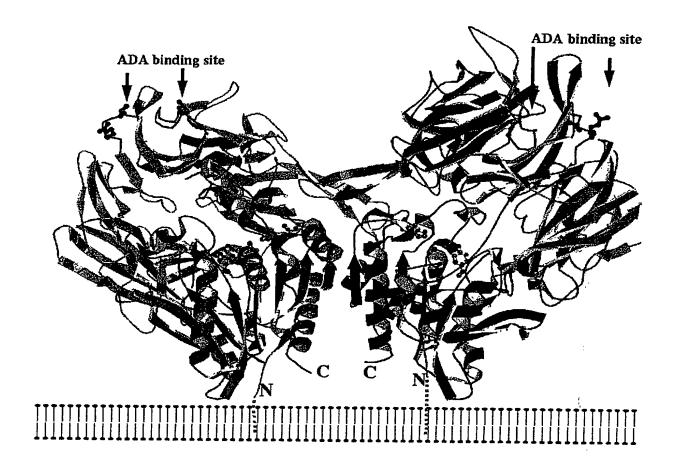


Figure 3 A

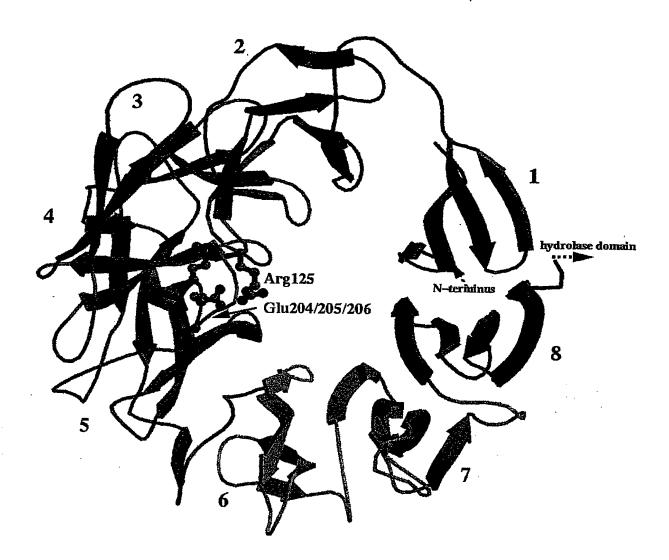


Figure 3B

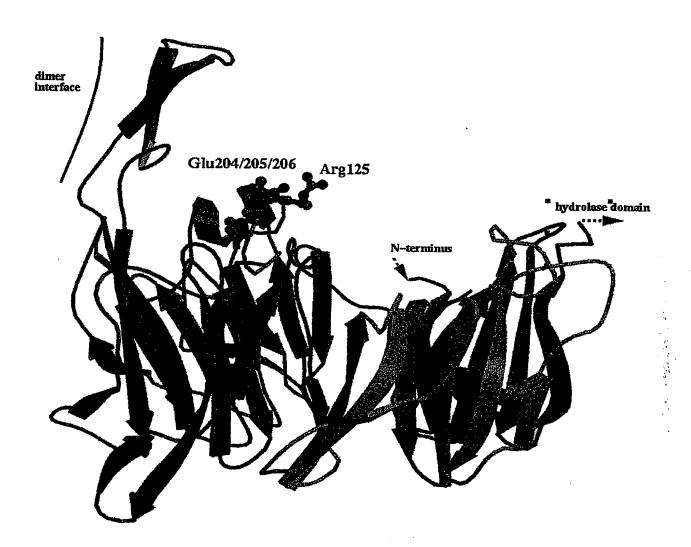


Figure 3C



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Figure 4

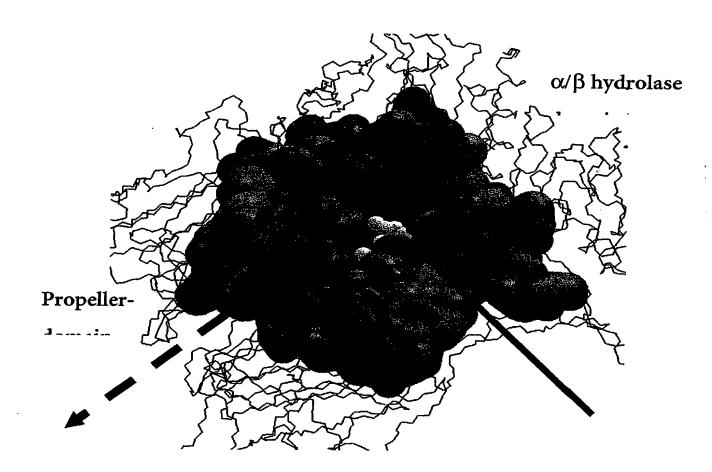
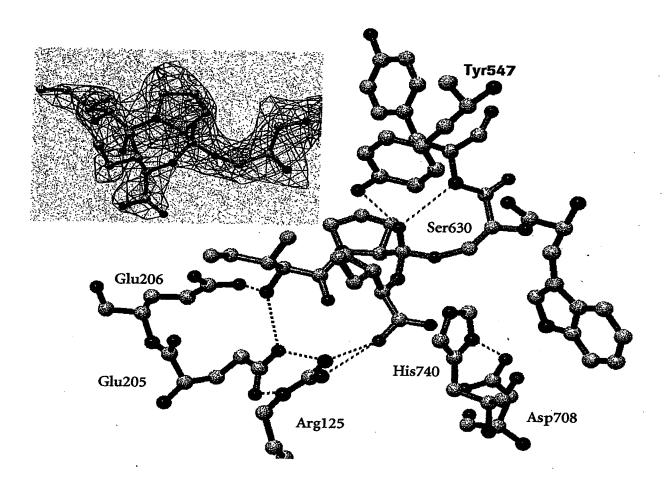


Figure 5



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